# Surface Science Division
# Fachverband Oberflächenphysik (O)

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# Overview of Invited Talks and Sessions

(Lecture halls H1, H2, H4, H6, H8, H11, H24, and H25; Poster P2 and P3)

## Invited Talks

| | | | | |
|---|---|---|---|---|
| O 7.4 | Mon | 11:15–11:45 | H11 | **Nanoimaging the electronic, plasmonic, and phononic structure and dynamics of 2D materials** — •Sarah King |
| O 8.1 | Mon | 10:30–11:00 | H24 | **Chiral reactions at surfaces elucidated by machine learning and enhanced sampling** — Raymond Amador, Enrico Trizio, Peilin Kang, Umberto Raucci, Hannah Bertschi, Marcella Iannuzzi, Jacob Wright, Roland Widmer, Oliver Gröning, Michele Parrinello, •Daniele Passerone |
| O 10.1 | Mon | 15:00–15:30 | H2 | **Probing coherent optical emission processes with ultrafast scanning electron microscopy** — •Albert Polman |
| O 10.5 | Mon | 16:15–16:45 | H2 | **Ultrafast exciton dynamics in momentum space** — Alexander Neef, Tommaso Pincelli, Lawson Lloyd, Shuo Dong, Samuel Beaulieu, Tania Mukherjee, Sebastian Hammer, Malte Selig, Dominik Christiansen, Andreas Knorr, Martin Wolf, Jens Pflaum, Laurenz Rettig, •Ralph Ernstorfer |
| O 15.1 | Mon | 15:00–15:30 | H24 | **Kondo and Yu-Shiba-Rusinov resonances: transport and coupling** — •Laëtitia Farinacci, Gelavizh Ahmadi, Gaël Reecht, Benjamin W. Heinrich, Contanstin Czekelius, Felix von Oppen, Katharina J. Franke |
| O 15.2 | Mon | 15:30–16:00 | H24 | **Electron delocalization in a 2D Mott insulator** — •Amadeo L. Vazquez de Parga, Cosme G. Ayani, Michele Pisarra, Iván M. Ibarburu, Clara Rebanal, Manuela Garnica, Fabián Calleja, Fernando Martín |
| O 15.3 | Mon | 16:00–16:30 | H24 | **Kondo or no Kondo, that is the question** — •Alexander Weismann, Neda Noei, Niklas Ide, Richard Berndt |
| O 15.4 | Mon | 16:30–17:00 | H24 | **Evidence for spinarons in Co atoms on noble metal (111) surfaces** — •Artem Odobesko |
| O 15.5 | Mon | 17:00–17:30 | H24 | **Spinarons: A new view on emerging spin-driven many-body phenomena in nanostructures** — •Samir Lounis |
| O 26.1 | Tue | 10:30–11:00 | H2 | **Attosecond Electron Microscopy** — •Peter Baum |
| O 27.7 | Tue | 12:00–12:30 | H4 | **Ultrafast electrochemistry beyond the RC time constant** — •Yujin Tong |
| O 30.5 | Tue | 11:30–12:00 | H11 | **Resonant molecular transitions in femtosecond second harmonic generation spectroscopy of Fe-porphyrin/Cu(001)** — •Andrea Eschenlohr, Rui Shi, Jinghao Chen, Ping Zhou, Uwe Bovensiepen, Wolfgang Hübner, Georg Lefkidis |
| O 31.3 | Tue | 11:00–11:30 | H24 | **Single molecule machines on surface** — •Francesca Moresco |
| O 57.3 | Wed | 11:00–11:30 | H2 | **Floquet engineering in black phosphorus** — •Changhua Bao, Shaohua Zhou, Benshu Fan, Michael Schüler, Teng Xiao, Hui Zhou, Zhiyuan Sun, Peizhe Tang, Sheng Meng, Wenhui Duan, Shuyun Zhou |
| O 61.3 | Wed | 11:00–11:30 | H11 | **Polaritons in two-dimensional materials and hybrids probed by electron beams** — •Nahid Talebi |
| O 62.5 | Wed | 11:30–12:00 | H24 | **On-Surface Synthesis with Hydrogen Atoms** — •Szymon Godlewski |
| O 64.1 | Wed | 15:00–15:30 | H2 | **Topological spin structures in two-dimensional van der Waals magnets and heterostructures** — •Stefan Heinze |

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| O 64.2 | Wed | 15:30–16:00 | H2 | **Ferromagnetic Order in 2D Layers of Transition Metal Dichlorides** — Andrea Aguirre, Andres Pinar, Diego Soler, Carmen Gonzalez-Orellana, Jon Ortuzar, Oleksandr Stesovych, Celia Rogero, Jose Ignacio Pascual, Pavel Jelinek, Maxim Ilyn, •Martina Corso |
| O 64.3 | Wed | 16:00–16:30 | H2 | **Tailoring spin lattice in van der Waals monolayer crystals** — •Ying-Shuang Fu |
| O 64.4 | Wed | 16:30–17:00 | H2 | **Spin excitations in 2D heterostructures from realistic fermionic models** — •António Costa |
| O 66.1 | Wed | 15:00–15:30 | H8 | **Unveiling the crucial role of kinetic modeling of gas flows in vacuum and fusion technologies** — •Christos Tantos, Thomas Giegerich |
| O 66.2 | Wed | 15:30–16:00 | H8 | **Advances in traceable vacuum and outgassing rate measurements** — •Matthias Bernien, Annas Bin Ali, Thomas Bock, Tom Rubin, Janez Setina, Perrin Waldock, Kirk Madison, Karl Jousten |
| O 68.9 | Wed | 17:00–17:30 | H24 | **On-Surface Synthesis of Porphyrins and BN-Substituted Carbon Scaffolds** — •Willi Auwärter |
| O 91.1 | Thu | 15:00–15:30 | H24 | **Infrared Nanoscopy and Tomography of Intracellular Structures** — Joachim Heberle, Katerina Kanevche, •Emmanuel Pfitzner, David Burr, Janina Drauschke, Andreas Elsaesser, Jacek Kozuch |
| O 91.2 | Thu | 15:30–16:00 | H24 | **Coherent Raman Imaging** — •Michael Schmitt, Juergen Popp |
| O 91.3 | Thu | 16:00–16:30 | H24 | **Sum Frequency Generation Microscopy of Electrochemical Interfaces** — •Steven Baldelli |
| O 100.1 | Fri | 10:30–11:00 | H24 | **Multidimensional Super-resolution Imaging: Wasting Light to Learn New Things** — •Steven Lee |
| O 100.2 | Fri | 11:00–11:30 | H24 | **MALDI mass spectrometry imaging: application examples ranging from food analysis to pharmaceutical research** — •Andreas Römpp |

## Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

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

## Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

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

## Invited Talks of the joint Symposium Progress and Challenges in Modelling Electron-Phonon Interaction in Solids (SYIS)

See SYIS for the full program of the symposium.

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

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

See SYFD for the full program of the symposium.

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

## Invited Talks of the joint Symposium Spins in Molecular Systems: Strategies and Effects of Hyperpolarization (SYMS)

See SYMS for the full program of the symposium.

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

## Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

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

## Sessions

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|---|---|---|---|---|
| O 1.1–1.4 | Sun | 16:00–18:00 | H3 | **Tutorial: How to Use NOMAD's Workflow Utilities to Improve Data Management and Facilitate Discovery in Materials Science (joint session O/TUT)** |
| O 2.1–2.3 | Sun | 16:00–18:15 | H10 | **Tutorial: Do it Yourself Guide for Simulating Complex Magnetism: From Theoretical Foundations to Hands-on Spin-dynamics (joint session O/TUT)** |
| O 3.1–3.1 | Mon | 9:30–10:15 | H24 | **Overview Talk Kerstin Volz** |
| O 4.1–4.10 | Mon | 10:30–13:00 | H4 | **Solid-Liquid Interfaces: Structure** |
| O 5.1–5.10 | Mon | 10:30–13:00 | H6 | **Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale I** |
| O 6.1–6.9 | Mon | 10:30–12:45 | H8 | **Oxides and Insulator Surfaces: Structure, Epitaxy and Growth** |
| O 7.1–7.8 | Mon | 10:30–12:45 | H11 | **Focus Session Ultrafast Electron Microscopy at the Space-Time Limit I** |
| O 8.1–8.9 | Mon | 10:30–13:00 | H24 | **Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation I** |
| O 9.1–9.8 | Mon | 10:30–12:30 | H25 | **Surface Reactions** |
| O 10.1–10.9 | Mon | 15:00–17:45 | H2 | **Focus Session Ultrafast Electron Microscopy at the Space-Time Limit II** |
| O 11.1–11.12 | Mon | 15:00–18:00 | H4 | **Electronic Structure of Surfaces: Spectroscopy, Surface States I** |
| O 12.1–12.11 | Mon | 15:00–17:45 | H6 | **Nanostructures at Surfaces I** |
| O 13.1–13.10 | Mon | 15:00–17:30 | H8 | **Organic Molecules on Inorganic Substrates: Adsorption and Growth** |
| O 14.1–14.12 | Mon | 15:00–18:00 | H11 | **2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)** |
| O 15.1–15.8 | Mon | 15:00–18:15 | H24 | **Focus Session Many-Body Phenomena in Nanomagnets: Kondo, Spinons, Spinarons and Beyond (joint session O/TT)** |
| O 16.1–16.12 | Mon | 15:00–18:00 | H25 | **Scanning Probe Techniques: Method Development** |
| O 17.1–17.12 | Mon | 18:00–20:00 | P2 | **Poster Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation** |
| O 18.1–18.7 | Mon | 18:00–20:00 | P2 | **Poster Focus Session Ultrafast Electron Microscopy at the Space-Time Limit** |
| O 19.1–19.2 | Mon | 18:00–20:00 | P2 | **Poster Surface Magnetism** |
| O 20.1–20.11 | Mon | 18:00–20:00 | P2 | **Poster Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale** |
| O 21.1–21.8 | Mon | 18:00–20:00 | P2 | **Poster Heterogeneous Catalysis** |
| O 22.1–22.6 | Mon | 18:00–20:00 | P2 | **Poster Surface Reactions** |
| O 23.1–23.21 | Mon | 18:00–20:00 | P2 | **Poster Ultrafast Electron Dynamics** |
| O 24.1–24.11 | Mon | 18:00–20:00 | P2 | **Poster Scanning Probe Techniques: Method Development** |
| O 25.1–25.1 | Tue | 9:30–10:15 | H24 | **Overview Talk Jörg Kröger** |
| O 26.1–26.9 | Tue | 10:30–13:00 | H2 | **Focus Session Ultrafast Electron Microscopy at the Space-Time Limit III** |
| O 27.1–27.9 | Tue | 10:30–13:00 | H4 | **Solid-Liquid Interfaces: Reactions and Electrochemistry I** |
| O 28.1–28.7 | Tue | 10:30–12:15 | H6 | **Graphene: Electronic Structure and Excitations (joint session O/HL)** |
| O 29.1–29.10 | Tue | 10:30–13:00 | H8 | **2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)** |
| O 30.1–30.8 | Tue | 10:30–12:45 | H11 | **Surface Magnetism** |
| O 31.1–31.9 | Tue | 10:30–13:00 | H24 | **Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation II** |
| O 32.1–32.9 | Tue | 10:30–12:45 | H25 | **Heterogeneous Catalysis I** |
| O 33.1–33.21 | Tue | 13:30–15:30 | P3 | **Poster Graphene: Electronic Structure and Excitations** |
| O 34.1–34.6 | Tue | 13:30–15:30 | P3 | **Poster Solid-Liquid Interfaces: Reactions and Electrochemistry** |
| O 35.1–35.4 | Tue | 13:30–15:30 | P3 | **Poster Solid-Liquid Interfaces: Structure** |
| O 36.1–36.8 | Tue | 13:30–15:30 | P3 | **Poster 2D Materials: Electronic Structure and Exitations (joint session O/HL)** |
| O 37.1–37.5 | Tue | 13:30–15:30 | P3 | **Poster 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)** |
| O 38.1–38.5 | Tue | 13:30–15:30 | P3 | **Poster 2D Materials: Stacking and Heterostructures (joint session O/HL)** |

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| O 39.1–39.6 | Tue | 14:00–15:30 | H4 | **Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules I** |
| O 40.1–40.6 | Tue | 14:00–15:30 | H6 | **Surface Dynamics** |
| O 41.1–41.5 | Tue | 14:00–15:15 | H8 | **Heterogeneous Catalysis II** |
| O 42.1–42.6 | Tue | 14:00–15:30 | H11 | **Electron-driven Processes** |
| O 43.1–43.7 | Tue | 14:00–15:45 | H24 | **Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale II** |
| O 44.1–44.3 | Tue | 18:00–20:00 | P2 | **Poster Oxides and Insulator Surfaces: Structure, Epitaxy and Growth** |
| O 45.1–45.18 | Tue | 18:00–20:00 | P2 | **Poster Spins on Surfaces at the Atomic Scale** |
| O 46.1–46.13 | Tue | 18:00–20:00 | P2 | **Poster Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties** |
| O 47.1–47.5 | Tue | 18:00–20:00 | P2 | **Poster Electron-driven Processes** |
| O 48.1–48.4 | Tue | 18:00–20:00 | P2 | **Poster Surface Dynamics** |
| O 49.1–49.11 | Tue | 18:00–20:00 | P2 | **Poster Nanostructures at Surfaces** |
| O 50.1–50.9 | Tue | 18:00–20:00 | P2 | **Poster Organic Molecules on Inorganic Substrates: Adsorption and Growth** |
| O 51.1–51.5 | Tue | 18:00–20:00 | P2 | **Poster Electronic Structure of Surfaces: Spectroscopy, Surface States** |
| O 52.1–52.5 | Tue | 18:00–20:00 | P2 | **New Methods: Experiment** |
| O 53.1–53.2 | Tue | 18:00–20:00 | P2 | **Poster Electronic Structure Theory** |
| O 54.1–54.1 | Tue | 18:00–20:00 | P2 | **Poster New Methods: Theory** |
| O 55.1–55.3 | Tue | 18:00–20:00 | P2 | **Poster Topology and Symmetry-protected Materials** |
| O 56.1–56.1 | Wed | 9:30–10:15 | H24 | **Overview Talk Pavel Jelinek** |
| O 57.1–57.9 | Wed | 10:30–13:00 | H2 | **Ultrafast Electron Dynamics I** |
| O 58.1–58.10 | Wed | 10:30–13:00 | H4 | **Solid-Liquid Interfaces: Reactions and Electrochemistry II** |
| O 59.1–59.10 | Wed | 10:30–13:00 | H6 | **Spins on Surfaces at the Atomic Scale I** |
| O 60.1–60.9 | Wed | 10:30–12:45 | H8 | **Plasmonics and Nanooptics: Fabrication, Characterization and Applications I** |
| O 61.1–61.8 | Wed | 10:30–12:45 | H11 | **2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)** |
| O 62.1–62.9 | Wed | 10:30–13:00 | H24 | **Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation III** |
| O 63.1–63.8 | Wed | 10:30–12:30 | H25 | **Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules II** |
| O 64.1–64.8 | Wed | 15:00–18:00 | H2 | **Focus Session Atomic Scale Investigation of Magnetic 2D Materials** |
| O 65.1–65.11 | Wed | 15:00–17:45 | H6 | **Solid-Liquid Interfaces: Reactions and Electrochemistry III** |
| O 66.1–66.10 | Wed | 15:00–18:00 | H8 | **Vacuum Science Technology: Theory and Applications** |
| O 67.1–67.11 | Wed | 15:00–17:45 | H11 | **Ultrafast Electron Dynamics II** |
| O 68.1–68.10 | Wed | 15:00–17:45 | H24 | **Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation IV** |
| O 69.1–69.10 | Wed | 15:00–17:30 | H25 | **Nanostructures at Surfaces II** |
| O 70.1–70.1 | Wed | 18:00–20:00 | P2 | **Poster Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules** |
| O 71.1–71.5 | Wed | 18:00–20:00 | P2 | **Poster Plasmonics and Nanooptics: Fabrication, Characterization and Applications** |
| O 72.1–72.13 | Wed | 18:00–20:00 | P2 | **Poster Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy** |
| O 73.1–73.10 | Wed | 18:00–20:00 | P2 | **Poster Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules** |
| O 74.1–74.7 | Wed | 18:00–20:00 | P2 | **Poster Metal and Semiconductor Substrates: Structure, Epitaxy and Growth** |
| O 75.1–75.1 | Wed | 18:00–20:00 | P2 | **Poster Focus Session Chemical Imaging for the Elucidation of Molecular Structure (joint session O/BP)** |
| O 76.1–76.3 | Wed | 18:00–20:00 | P2 | **Poster Focus Session Atomic Scale Investigation of Magnetic 2D Materials** |
| O 77.1–77.3 | Wed | 18:00–20:00 | P2 | **Poster Vacuum Science Technology: Theory and Applications** |
| O 78.1–78.1 | Thu | 9:30–10:15 | H24 | **Overview Talk Manish Garg** |
| O 79.1–79.8 | Thu | 10:30–12:30 | H2 | **Ultrafast Electron Dynamics III** |
| O 80.1–80.8 | Thu | 10:30–12:30 | H4 | **Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties I** |

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|---|---|---|---|---|
| O 81.1–81.8 | Thu | 10:30–12:30 | H6 | **Heterogeneous Catalysis III** |
| O 82.1–82.8 | Thu | 10:30–12:30 | H8 | **Plasmonics and Nanooptics: Fabrication, Characterization and Applications II** |
| O 83.1–83.8 | Thu | 10:30–12:30 | H11 | **2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)** |
| O 84.1–84.5 | Thu | 10:30–13:00 | H24 | **Gerhard Ertl Young Investigator Award Competition** |
| O 85.1–85.9 | Thu | 10:30–12:45 | H25 | **New Methods: Theory** |
| O 86.1–86.10 | Thu | 15:00–17:30 | H2 | **Electronic Structure of Surfaces: Spectroscopy, Surface States II** |
| O 87.1–87.10 | Thu | 15:00–17:30 | H4 | **Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy I** |
| O 88.1–88.11 | Thu | 15:00–17:45 | H6 | **2D Materials: Stacking and Heterostructures (joint session O/HL)** |
| O 89.1–89.11 | Thu | 15:00–17:45 | H8 | **Metal and Semiconductor Substrates: Structure, Epitaxy and Growth** |
| O 90.1–90.10 | Thu | 15:00–17:30 | H11 | **Spins on Surfaces at the Atomic Scale II** |
| O 91.1–91.7 | Thu | 15:00–17:30 | H24 | **Focus Session Chemical Imaging for the Elucidation of Molecular Structure I (joint session O/BP)** |
| O 92.1–92.13 | Thu | 15:00–18:15 | H25 | **Electronic Structure Theory** |
| O 93 | Thu | 19:00–19:30 | H1 | **Members' Assembly** |
| O 94 | Thu | 19:30–20:30 | H1 | **Post Deadline Session** |
| O 95.1–95.1 | Fri | 9:30–10:15 | H24 | **Overview Talk Kai Rossnagel** |
| O 96.1–96.10 | Fri | 10:30–13:00 | H4 | **Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy II** |
| O 97.1–97.8 | Fri | 10:30–12:30 | H6 | **Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties II** |
| O 98.1–98.8 | Fri | 10:30–12:30 | H8 | **Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules** |
| O 99.1–99.10 | Fri | 10:30–13:00 | H11 | **Ultrafast Electron Dynamics IV** |
| O 100.1–100.7 | Fri | 10:30–12:45 | H24 | **Focus Session Chemical Imaging for the Elucidation of Molecular Structure II (joint session O/BP)** |
| O 101.1–101.7 | Fri | 10:30–12:15 | H25 | **Topology and Symmetry-protected Materials (joint session O/TT)** |
| O 102.1–102.1 | Fri | 13:15–14:00 | H1 | **Closing Talk Andreas Heinrich** |

## Members' Assembly of the Surface Science Division

Thursday 19:00–19:30 H1

## O 1: Tutorial: How to Use NOMAD's Workflow Utilities to Improve Data Management and Facilitate Discovery in Materials Science (joint session O/TUT)

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

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

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

Time: Sunday 16:00–18:00 Location: H3

**Tutorial** O 1.1 Sun 16:00 H3
**FAIR-data management with the NOMAD infrastructure: Core functionalities** — •Joseph F. Rudzinski — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

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

**Tutorial** O 1.2 Sun 16:30 H3
**Using NOMAD's API for project management** — •Nathan Daelman — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

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

**Tutorial** O 1.3 Sun 17:00 H3
**Creating custom entries in NOMAD using yaml schema and ELN integration** — •Andrea Albino — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

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

**Tutorial** O 1.4 Sun 17:30 H3
**Creating custom workflow entries in NOMAD to link multiple uploads** — •Bernadette Mohr — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

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

## O 2: Tutorial: Do it Yourself Guide for Simulating Complex Magnetism: From Theoretical Foundations to Hands-on Spin-dynamics (joint session O/TUT)

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

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

**Tutorial** O 2.1 Sun 16:00 H10
**Derivation of the spin-lattice Hamiltonian: Heisenberg, beyond Heisenberg, DMI, nematic exchange** — •Hiroshi Katsumoto — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52428 Jülich, Germany

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

**Tutorial** O 2.2 Sun 16:45 H10

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

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

**Tutorial** O 2.3 Sun 17:30 H10

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

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

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

## O 3: Overview Talk Kerstin Volz

Time: Monday 9:30–10:15 Location: H24

**Topical Talk** O 3.1 Mon 9:30 H24

**Insights in real and electronic structure of interfaces by electron microscopy** — •Kerstin Volz — Philipps-Universität Marburg, Center for Quantum Materials and Sustainable Technology (mar.quest) and Department of Physics, Hans Meerwein Str., 35032 Marburg, Germany

Internal interfaces between materials are decisive for the functionality of many devices. Hence, an understanding of the atomic as well as electronic structure across interfaces is essential. Electron microscopy can give insights into these properties from Angstrom to several micrometer length scales. With examples from semiconductors, batteries and 2D materials I will show, how Scanning Transmission Electron Microscopy (STEM) can be used to gain the desired information. Thereby, a focus will be on state of the art and quantitative techniques like 4-dimensional STEM, where real as well as momentum space are mapped to derive information on composition, but also on electric fields. These properties will be correlated to fundamental excitations of the charge carrier system at interfaces, e.g., excitons, probed by monochromated Electron Energy Loss Spectroscopy (EELS).

## O 4: Solid-Liquid Interfaces: Structure

Time: Monday 10:30–13:00 Location: H4

O 4.1 Mon 10:30 H4

**The Impact of the Gold Interface on the Structure and Properties of Aqueous Sodium Citrate Solution** — •Elspeth Smith and Marialore Sulpizi — Ruhr-Universität Bochum, Bochum, Germany

Gold nanoparticles (AuNPs) are used widely, with many commercial applications due to their being well suited for catalysis. Owing to the method of production/stabilisation, AuNPs are often suspended in a solution of aqueous sodium citrate, a system with complicated interplays which we seek to elucidate in this work.

Through the use of a previously developed polarisable gold model we have performed all atom classical molecular dynamics simulations of a variety of systems and concentrations of sodium citrate solution, employing the SPC/E water model and a CHARMM based citrate model, with and without a gold interface. In order to better understand the dual effect of both the gold interface and sodium citrate on the water's structure, we employ a number of widely used order parameters for water. As the structure of water in close proximity to AuNPs is difficult to observe experimentally and has possibly large applications for their use in catalysis, we hope to obtain a better understanding of this elusive phenomenon.

O 4.2 Mon 10:45 H4

**Rationalizing the “Anomalous” Electrochemical Stark Shift of CO at Pt(111) Through Vibrational Spectroscopy and Density-Functional Theory Calculations** — •Elias Diesen[1], Mehmet Ugur Coskun[2], Sergio Díaz-Coello[2], Vanessa J. Bukas[1], Julia Kunze-Liebhäuser[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Department of Physical Chemistry, University of Innsbruck, Austria

We employ infrared reflection absorption spectroscopy (IRRAS) and first-principles density-functional theory (DFT) to revisit the reported “anomalous” negative Stark shift of the CO stretch frequency at Pt(111) in aqueous electrolyte [1]. Our measurements confirm the existence of a potential region with negative Stark shift around 0.5 V vs. RHE at sufficiently high CO concentration in the electrolyte. As these are exactly the same conditions for the occurrence of a phase transition from a $(2 \times 2)$–3CO to a $(\sqrt{19} \times \sqrt{19})$R23.4°–13CO adsorbate structure [2], we explicitly compute the Stark shift for these two phases using DFT. Neither phase exhibits a negative Stark shift, but the absolute stretch frequencies of atop CO in the two structures are slightly shifted with respect to each other. Remeasuring IRRAS with high resolution indeed reveals a doublet character of the absorption band in the potential region corresponding to the negative Stark shift. Separate fits of the two components then yield positive Stark shifts in quantitative agreement with the calculated values.

[1] Stamenkovic et al., J. Phys. Chem. B 109, 678 (2005); [2] Wei et al., J. Phys. Chem. C 125, 3066 (2021)

O 4.3 Mon 11:00 H4

**Adatom Dynamics at Water/Pt(111) Interface from Ab Initio Free Energy Analysis** — •Sung Sakong[1], Jonas Lindner[2], Ulrich Ross[3], Michael Seibt[3], Christian Jooss[2], and Axel Gross[1] — [1]Institute of Theoretical Chemistry, Ulm University, 89081 Ulm, Germany — [2]Institute of Materials Physics, University of Göttingen, 37077 Göttingen, Germany — [3]4th Institute of Physics Solids and Nanostructures, University of Göttingen, 37077, Göttingen, Germany

Recent electron diffraction experiments investigated the local structures of the water/Pt(111) interface, a selected model system for investigating the structural properties of the electric double layer (EDL). The reconstructed phase signals of the diffraction data yield the time average of the interface structures with Angstrom resolution and observe the static Pt lattice and dynamic particles above the lattice. Since the time-averaged signals from experiments are often challenging to relate to the corresponding atomic structures of dynamic particles, we probe the interface structure by including Pt adatoms using the ab initio molecular dynamics (AIMD) method. The free energy of Pt adatoms is analyzed by including the vibrational entropy calculated from the AIMD trajectories using the two-phase thermodynamics method. While the dynamics of water molecules are captured within the AIMD trajectories, the relatively slow Pt adatom dynamics are estimated by a free energy analysis, Blue Moon ensemble sampling. By comparing the Water/Pt(111) and Vacuum/Pt(111) models, we will discuss the role of surrounding water molecules and try to relate the model EDL configurations to the experimental findings.

O 4.4 Mon 11:15 H4

**Effect of the damping function in dispersion corrected density functional theory on properties of liquid water** — •Knut Nikolas Lausch[1,2], Redouan El Haouari[1,2], Daniel Trzewik[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

Accounting for non-local dispersion interactions is essential to achieve chemical accuracy when applying approximate density functional theory (DFT) to large molecular or condensed systems. A popular approach is to add a damped correction potential, based on the London formula, after convergence. Damping is required to avoid the diverging short-range behavior of the London formula and double counting of interactions treated locally by the exchange-correlation (xc) functional. Often two forms of damping, known as zero- and Becke-Johnson-damping, are employed and it is generally assumed that the choice has only a minor impact on performance even though the resulting correction potentials differ quite dramatically. Here, we demonstrate that the choice of damping function can have a major impact on properties obtained from molecular dynamics simulations of liquid water suggesting that the significance of damping in dispersion corrected DFT needs to be reevaluated.

O 4.5 Mon 11:30 H4

**Elucidating the double layer structure of protic ionic liquid electrolytes for next-generation fuel cells** — •Christian Rodenbücher, Yingzhen Chen, Federico Parisi, Piotr M. Kowalski, and Carsten Korte — Forschungszentrum Jülich GmbH, Institute of Energy Technologies (IET-3 & IET-4), 52425 Jülich, Germany

Polymer electrolyte membrane fuel cells (PEMFCs) are the backbone of a future hydrogen-based renewable energy system. Increasing their operation temperature to 100–160 °C would allow for a simpler water management and the use of waste heat. In this temperature range, conventional proton conducting polymers such as Nafion are not applicable, since they rely on the presence of water. Hence, we study immidazolium-based protic ionic liquids, which provide a high thermal and chemical stability and a high proton conductivity. We present experimental investigations using impedance spectroscopy, infrared spectroscopy, and atomic force microscopy combined with atomistic simulations by molecular dynamics and density functional theory. Our results reveal that depending on the electrode charge, a dense layered structure of alternating anion and cation layers is formed. Upon the addition of water, which is naturally produced during fuel cell operation, the structuring becomes distorted resulting in the accumulation of water at the interface and the increase of the onset potential of the oxygen reduction reaction. Our findings illustrate that the kinetics of the fuel cell reactions is influenced not only by bulk properties of the electrolyte but also by the adsorption at the electrode, which may be tuned by designing ionic liquids with bespoke properties.

O 4.6 Mon 11:45 H4

**Polarizable model of graphite and its applications to nanotechnology** — Krishan Kanhaiya[1], Hendrik Heinz[2], and •Marialore Sulpiziz[3] — [1]Ruhr-Universität Bochum — [2]University of Colorado Boulder — [3]Ruhr-Universität Bochum

Graphitic materials are of significant importance in the research and industrial community due to their tunable electrical conductivity, band gap, thermal property and high strength to mass ratio. They are used in battery or fuel cells as electrodes, refractory material, lubricant, aerospace, water purification, and bio-sensing etc.. We present a realistic, all-atom polarizable model of graphite with flexible dummy electrons to model the polarizable nature of electron cloud, similar to the approach which was used to describe image charge effects for ions approaching metal surfaces. The models predict density, lattice parameters, surface energy, hydration energy, water contact angle and elastic constants within 1%, 1%, 5%, 5%, 5% and ~15 % respectively as per the Interface Force Field protocol. Additionally, the model also reproduces experimental and DFT data on binding energies and profiles for cations , anions and neutral molecules (water, amino acids, and organic molecules). We further discuss friction coefficient across the graphene surface and nanotubes in order to model flow characteristics of water over such surfaces . An accurate description of such systems is key to design improved functional materials and devices for water desalination and blue energy (electric energy from salinity gradient in two different electrolyte solutions).

O 4.7 Mon 12:00 H4

**Elucidating the interaction of small organic pollutants at ice surfaces with sum-frequency generation spectroscopy** — •Gurivi reddy Yettapu[1,2], Luca B. Manning[2], and Jenee D. Cyran[2] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]Boise State University, Boise, USA

Small organic pollutants interacting with ice and water surfaces in the troposphere are relevant for atmospheric compositional changes.[1] Their interactions with hexagonal basal-plane oriented single crystalline ice have been scarcely revealed.[2] Methanol and acetone are two smallest organic molecules that interact differently with single crystalline ice surfaces. Herein, we probed their direct interaction on ice and water interfaces with surface-specific, mode selective sum-frequency generation spectroscopy. Our results show significant difference in the frequency of H-bonding O-H oscillators of water molecules present at the ice interface.[3] The distinct behavior of the adsorption of these molecules could explain their relevant atmospheric compositions. [1] F. Dominé and P. B. Shepson, Science, 297, 1506-1510 (2002). [2] J. D. Cyran et al., Angew. Chem. Int. Ed., 58, 3620-3624 (2019). [3] G. R. Yettapu et al., Faraday Discussions, just accepted (2024).

O 4.8 Mon 12:15 H4

**Exploring Charged Aqueous Interfaces with Depth-Resolved SFG/DFG Vibrational Spectroscopy** — •Sarabjeet Kaur, Álvaro Díaz Duque, Alexander Fellows, Martin Wolf, and Martin Thämer — Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society

Charged aqueous interfaces are crucial in biological, atmospheric, and chemical processes, where surface electric fields influence ion distributions and interfacial dynamics. Water mediates these interactions, with effects spanning nanometers. The Gouy-Chapman (GC) model and variants describe ion distributions but oversimplify water as a continuous medium, neglecting molecular-level behaviors like impact of structure, orientation, and hydrogen-bonding dynamics. This omission leaves important aspects of interfacial phenomena unexamined. We address these gaps using depth-resolved vibrational spectroscopy combining phase-resolved sum- and difference-frequency generation (SFG and DFG). This technique reveals depth-dependent water responses and connects electric potential anisotropy with molecular reorientation. Our findings identify two distinct interfacial layers, challenging the single-layer GC model. Spectral analysis shows structural differences between the compact and diffuse layers. Additionally, concentration-dependent studies highlight discrepancies between the observed decay length of orientational anisotropy and the predicted Debye length. These results underscore the limitations of the GC variant model and continuum solvent approaches in capturing water's molecular-level behavior at charged interfaces.

O 4.9 Mon 12:30 H4

**Resolving the water structure at iron-oxide/water interface** — •Harsharan Kaur[1], Moritz Zelenka[1,2], and Ellen Backus[1,2] — [1]University of Vienna, Faculty of Chemistry, Institute of Physical Chemistry, Währinger Str. 42, 1090 Vienna, Austria — [2]University of Vienna, Vienna Doctoral School in Chemistry (DoSChem), Währinger Str. 42, 1090 Vienna, Austria

Among different iron-oxide polymorphs, Fe3O4 is utilized as a catalyst for industrial-gas shift and photocatalytic water splitting reactions, where it often encounters water. [1] Fe3O4 surface is known to protonate and deprotonate on contact with pH-variant aqueous media. [1] However, less is known about the interfacial species and their molecular orientation under ambient condition. Herein, we explore these attributes at the magnetite-water interface as function of solution pH with macroscopic amount of water. Magnetite films of ~50 nm thick were prepared using magnetron sputtering and were found to sustain Fe3O4 phase combined with FeO or $\gamma$-Fe2O3 state. The interface was examined with SFG vibrational spectroscopy. Due to its selection rule, a vibrational spectrum of only the interfacial species is obtained in case of centrosymmetric bulk materials like Fe3O4 and water. We observed a pH-dependent variation in the H-bonding strength of the interfacial water molecules and the presence of Fe-OH groups at alkaline pH. Besides, the water orientation varies with pH. By comparing the results for Fe3O4 to Fe2O3, a detailed molecular picture of interfacial water at these relevant iron oxides will be presented. [1]. Z. Bielan, S. Dudziak, A. Kubiak, E. Kowalska, Appl. Sci. 11 (2021) 10160.

O 4.10 Mon 12:45 H4

**Structural and dynamical properties of the Solvated Electron From Ab Initio Molecular Dynamics Simulations** — •Anna Karolyna Macieira Silva Gomes and Marialore Sulpizi — Ruhr-University Bochum, Bochum, Germany

The solvated electron is a critical species in plasma/liquid and plasma/solid/liquid interfaces, serving as the primary reducing agent generated at plasma electrodes in contact with liquids. Recently, experimental studies have revealed differences in the properties of solvated electrons formed via plasma compared to other methods, such as water radiolysis. It has been proposed that the unique conditions at plasma interfaces, including electric fields, may alter the electron's solvation properties.

Despite extensive investigations into solvated electrons, their behavior in the presence of electric fields remains unexplored. This project employs atomistic molecular dynamics simulations to explore the influence of electric fields on the structure and dynamics of solvated electrons in aqueous solutions. Ab Initio Molecular Dynamics (AIMD), utilizing hybrid functionals, have been shown to offer a accurate approach to modeling the electronic properties of this system, while remaining computationally feasible for capturing relevant time and length scales.

## O 5: Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale I

Time: Monday 10:30–13:00 Location: H6

O 5.1 Mon 10:30 H6

**Simulated tip-enhanced Raman scattering fingerprints of doped triangulenes** — •Orlando Silveira[1,2], Markus Junttila[1], Shawulienu Kezilebieke[2,3], and Adam Foster[1,4] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Department of Physics, Nanoscience Center, University of Jyvaskyla, Jyvaskyla, Finland — [3]Department of Chemistry, University of Jyvaskyla, Jyvaskyla, Finland — [4]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa, Japan

Triangulenes are organic molecules promising for future applications in spintronics technologies, and fine tunning their electronic and magnetic properties will only extend the potential applications. A reliable possibility for such control is doping the triangulenes with different atoms such as nitrogen and boron. Usually, the reaction yield of triangulenes is quite small, and it is prohibitive to use techniques with high cross section such as Raman to chemically characterize the triangulenes. In the other hand, scanning probe microscopy (SPM) techniques have been successfully used for their structural characterization. In this work, we propose that the tip-enhanced Raman scattering (TERS) can be used for simultaneous chemical and structural characterization of the triangulenes. Our work offers a new perspective to study the triangulenes, as their vibrational properties have not yet been fully investigated, and the same simulation protocol used here can be applied to any other type of molecule.

O 5.2 Mon 10:45 H6

**Plasmon-induced reaction in hydrogen-bonded molecular networks studied by laser-coupled STM** — •Youngwook Park, Adnan Hammud, Martin Wolf, and Akitoshi Shiotari — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Hydrogen-bonded molecular networks are widely found in natural systems and play an important role in the development of functional molecular assemblies. Understanding chemical reactions within these networks requires molecular-level spatial resolution, which is challenging for photochemical studies. In this talk, we present a plasmon-induced reaction in 2D hydrogen-bonded assemblies, studied with a laser-coupled scanning tunneling microscope (STM). We investigated triphenylene-2,6,10-tricarboxylic acid forming a honeycomb network on Au(111) through hydrogen bonds. Our findings showed that photo-induced deformation of the network was localized to a few molecules beneath the Ag tip under visible laser illumination. In contrast, a PtIr tip, which lacks plasmonic activity in the visible range, failed to trigger the reaction. By varying the laser wavelength, we identified that non-thermal (hot) electrons generated by plasmons mediate the reaction. This was confirmed by initiating the reaction with non-thermal electrons from the STM tip without laser irradiation. Our results highlight the potential of plasmonic STM tips for precise control over molecular network structure and reactivity.

O 5.3 Mon 11:00 H6

**Motion of molecular motors on ultra-thin NaCl islands on Cu(111)** — •Monika Schied[1,2], Grant J. Simpson[1], Ken Kolar[1], Dongdong Liu[3], James M. Tour[3], and Leonhard Grill[1] — [1]University of Graz, Austria — [2]CNR-IOM, Italy — [3]Rice University, USA

Molecular motors are designed to overcome nature's random motion by converting external energy into controlled, uni-directional rotation. Studying them on a solid surface can be advantageous, as it offers confinement in two dimensions, making it easier to observe the directionality of their motion. In previous studies on metallic surfaces, indeed uni-directional rotation has been observed [1]. However, the activation of the motor functionality is likely suppressed due to the hybridisation of the molecular orbitals with the electron bath of the metal. In order to preserve the inherent electronic structure of the free molecule, we studied Feringa-type motors adsorbed on ultra-thin NaCl layers on Cu(111), which electronically decouples them from the metal substrate, while still permitting measurements with the low-temperature scanning tunnelling microscope (LT-STM). We excited the molecules with UV light, which – in contrast to voltage pulses – acts remotely without altering the local potential energy landscape with the STM tip. In this way, we could induce the motion of individual molecules.

[1] M. Schied et.al., ACS Nano 2023, 17, 4, 3958-3965

O 5.4 Mon 11:15 H6

**Triggering chemical reactions in single molecules with ultrashort THz pulses** — •Niklas Friedrich, Carmen Roelcke, Tzu-Chao Hung, Yaroslav Gerasimenko, Rupert Huber, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany

In lightwave-driven scanning tunnelling microscopy (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. This allows unravelling the dynamics of quantum systems in pump-probe experiments with atomic spatial and femtosecond temporal resolution [1].

Here, we show that LW-STM can be used to trigger chemical reactions on ultrashort timescales. We study free-base naphthalocyanine molecules (H2Nc) on 2ML NaCl on Cu(111). In DC-biased experiments, this system switches between different tautomers upon injection of high-energy tunnelling electrons [2]. 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, even a stepwise deprotonation of the molecule is activated by the ultrashort laser pulses when increasing the voltage transient beyond a threshold value.

[1] Roelcke et al. Nat. Photon. 18, 595-602 (2024) [2] Liljeroth et al. Science 317, 1203-1206 (2007)

O 5.5 Mon 11:30 H6

**Spatial coherent phonon spectroscopy on 2H-MoTe$_2$ using THz-STM** — •Vibhuti Rai, Junyoung Sim, Florian Faaber, Sergey Trishin, Nils Bogdanoff, Tom Seifert, Tobias Kampfrath, Christian Lotze, and Katharina J. Franke — Freie Universität Berlin, Department of Physics, Arnimallee 14,14195 Berlin, Germany

Scanning tunneling microscopy (STM) offers subnanometer spatial resolution. However, it lacks the temporal resolution required to investigate the dynamics of various elementary excitations such as phonons. By integrating STM with a pump-probe scheme that utilizes two terahertz (THz) pulses acting as transient bias voltages, subpicosecond time resolution can be achieved [1,2]. Here, we demonstrate that our custom-built THz setup, combined with an STM operating at 5K in an ultra-high vacuum, can be used to excite and detect lattice vibrations on the surface of 2H-MoTe$_2$. The time-resolved spectrum shows a long-lasting oscillatory signal that is sensitive to surface defects [3,4]. Fourier analysis reveals the presence of two prominent excitation modes. We correlate the excited modes with coherent phonons. The spatial variation of such coherent phonon spectroscopy further reveals that one of the two excited modes are enhanced by the surface defects.

[1] Cocker, et al. Nat. Photon. 7, 620-625 (2013)
[2] Yoshida et al. ACS Photonics 6, 6, 1356-1364 (2019)
[3] Liu et al. Sci. Adv. 8, eabq5682 (2022)
[4] Roelcke et al. Nat. Photon. 18, 595-602 (2024)

O 5.6 Mon 11:45 H6

**Charge Transfer in Lightwave-Driven Scanning Tunneling Microscopy** — •Nils Krane, Jonas Allerbeck, Laric Bobzien, S. Eve Ammerman, and Bruno Schuler — Empa - nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland

Lightwave-driven STM is a promising technique for exploring ultrafast charge-state dynamics at nanoscale. The tip electrode of the STM provides spatial resolution at the single-atom level, while single-cycle lightwave pulses supply an ultrafast voltage source at GHz to multi-THz frequencies that injects charge carriers to the system. In contrast to optical far-field measurements, the STM tip interacts with the investigated system also between the pulses where the applied voltage is low. This allows for ultrafast back tunneling of electrons from an excited charge state via discharging to the tip electrode, resulting in zero net current. Equal magnitude of forward and backward tunneling hence quenches the time-integrated charge rectification and imposes a major challenge on investigating ultrafast nanoscale charge dynamics. In this talk, I discuss the consequences of back tunneling for lightwave-driven STM and time-domain pump-probe techniques, at the example of picosecond charge-state lifetimes related to selenium vacancies in WSe$_2$ studied with THz-STM. I outline pathways to overcome this challenge by utilizing effects such as the Franck-Condon blockade or spin multiplicity for the promotion of unidirectional charge transport. A theoretical model based on the master equation, accurately reproduces the time-dependent tunneling processes observed in the experiments.

O 5.7 Mon 12:00 H6

**Ultrafast Coulomb blockade in an atomic-scale quantum dot** — Jonas Allerbeck[1], •Laric Bobzien[1], Nils Krane[1], S. Eve Ammerman[1], Daniel E. Cintron Figueroa[2], Joshua Robinson[2,3], and Bruno Schuler[1] — [1]Empa - nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland — [2]Department of Chemistry, The Pennsylvania State University, University Park, 16802, PA, USA — [3]Department of Physics and Department of Materials Science and Engineering, The Pennsylvania State University, University Park, 16802, PA, USA.

Controlling electron dynamics at optical clock rates is a fundamental challenge in lightwave-driven nanoelectronics. At the example of individual selenium vacancies (Vac$_{\mathrm{Se}}$) in few-layer tungsten diselenide (WSe$_2$), which are prototypical atomic-scale quantum dots with localized defect states, I present ultrafast charge transfer in the time domain using lightwave-driven scanning tunneling microscopy (LW-STM). Layer-dependent decoupling of Vac$_{\mathrm{Se}}$ in WSe$_2$ varies the average charge-state lifetime of defect states from 1.2 ps (1L) to 3 ns (4L), showing an unexpected sub-exponential. Picosecond terahertz (THz) source pulses, focused onto the picocavity of the STM, control and read the charge state of individual Vac$_{\mathrm{Se}}$ quantum dots. THz pump-THz probe time-domain sampling of the defect charge population captures atomic-scale snapshots of the transient Coulomb blockade, a signature of charge transport via quantized defect states. These results open new avenues for exploring charge dynamics and lightwave-driven electronics at the space-time limit.

O 5.8 Mon 12:15 H6

**THz Pulse induced Luminescence in a Scanning Tunneling Microscope** — •Kurt Lichtenberg, Johannes Schust, Felix Huber, Ines Hartkopf, Susanne Baumann, and Sebastian Loth — University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany

Light-matter interaction at the atomic scale lies at the heart of many processes in nature and technology, ranging from light harvesting to quantum communication applications. But experimental tools to access the respective dynamics at this scale with sufficient time resolution are rare.

Here we show a proof-of-concept combination of the ultrafast time resolution of THz scanning tunneling microscopy (THz STM) with tunneling-induced light emission at the atomic scale (Scanning Tunneling Luminescence).

We use intense sub-cycle THz pulses to excite plasmons in the tunnel junction consisting of a gold tip and a bare silver sample. We find that THz-induced voltage transients ignite luminescence in ultrashort time intervals within a fraction of a single period of the THz pulse that was used for the excitation. These ultrafast luminescence bursts can be used to sample the waveform of a second THz pulse with femtosecond time resolution.

This work contributes to a new line of methodology, that can probe the rich dynamics of light emission from single atoms and molecules.

O 5.9 Mon 12:30 H6

**Ultrafast manipulation of charge-density wave order with THz-STM** — Shaoxiang Sheng[1,2], Kurt Lichtenberg[1], Susanne Baumann[1], and •Sebastian Loth[1,3] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart, Stuttgart, Germany

Charge-density wave (CDW) materials present unique opportunities for exploring the interplay between structural distortions and the collective dynamics of complex electronic phases at the atomic scale. We use terahertz spectroscopy in the scanning tunneling microscope (THz-STM) to investigate charge-order dynamics in the prototypical CDW materials 2H-NbSe$_2$ and 1T-TaS$_2$. By employing tip-enhanced terahertz electric fields, we directly excite phase dynamics of the charge order and probe their local electronic response by terahertz-induced electron tunneling. Our measurements show that the incommensurate CDW of NbSe$_2$ features slow phase dynamics in the proximity of defects [1], whereas the commensurate CDW of TaS$_2$ exhibits fast reconfigurations within individual domains. The presented spatially resolved dynamics of CDWs demonstrate how atomically localized THz excitation can be leveraged to manipulate electronic states with femtosecond temporal precision, offering insights into the fundamental mechanisms of electronic or structural phase transitions in different materials.

[1] S. Sheng, et al., Nat. Phys. 20, 1603 (2024).

O 5.10 Mon 12:45 H6

**Tracking phonon-induced electronic dynamics on atomic scale with ultrafast tunnelling spectroscopy** — Carmen Roelcke, Lukas Kastner, Maximilian Graml, Jan Wilhelm, Jascha Repp, Rupert Huber, and •Yaroslav Gerasimenko — Department of

Physics and Regensburg Centre for Ultrafast Nanoscopy, University of Regensburg, 93040 Regensburg, Germany

Atomic-defect-based quantum systems in monolayers and moiré heterostructures of 2D materials have attracted huge interest for their qubit and single-photon emission functionalities, but directly observing the interplay of their electronic structure with elementary excitations remained a long-held dream.

We directly resolve in space, time and energy how spin-orbit-split bound states of an individual Se vacancy – an atomic single-photon emitter – evolve under coherent lattice vibrations in moiré-distorted $WSe_2$ using lightwave-driven scanning tunnelling spectroscopy [1]. We selectively launch a drum phonon mode with a THz pulse coupled to the tip and take ultrafast snapshots of electronic spectrum on atomic scales faster than a vibration period. Such ultrafast tunnelling spectra reaching ∼300 fs temporal resolution reveal transient energy shifts of the lower vacancy state by up to 40 meV, depending on the amplitude and phase of the coherent lattice vibration. We discuss how THz fields can couple via the Coulomb interactions to the drum mode, and how the interplay of Se-W bonds distortion and image charge renormalization affect the energy levels of the vacancy.

[1] C. Roelcke et al., Nat. Photon. 18, 595-602 (2024)

## O 6: Oxides and Insulator Surfaces: Structure, Epitaxy and Growth

Time: Monday 10:30–12:45 Location: H8

O 6.1 Mon 10:30 H8

**Characterizing Approximants of Oxide Quasicrystals with a Novel Geometric Approach** — •Martin Haller, Sebastian Schenk, Stefan Förster, and and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Oxide quasicrystals (OQCs) are aperiodic 2D oxide films exhibiting dodecagonal symmetry, which are grown on hexagonal metal substrates. This dodecagonal symmetry arises from a square-triangle-rhombus tiling, derived from Ba, Sr, or Eu hosted within a Ti-O network [1]. Approximants are periodic structures composed of the same tiling elements, thus exhibiting a close structural relationship to the OQC. Variations in stoichiometry lead to the emergence of different approximant structures, ranging from simple tilings with a triangle:square:rhombus frequency ratio of 4:2:0 to more complex configurations such as the 60:22:8 approximant [2]. In this presentation, we will introduce newly discovered approximant phases identified in the Sr-Ti-O/Pd(111) and Eu-Ti-O/Pd(111) systems through STM and LEED. Specifically, we will discuss two hexagonal approximants with tiling frequency ratios of 20:3:6 and 8:0:3, as well as an oblique 10:3:2 approximant. Additionally, we will apply a novel geometric approach for characterizing the tilings derived from STM data [3]. This innovative method provides a measure in a 4D hyperspace for classifying the relationship of approximants to the parent OQC.

[1] Schenk et al., Nature Communications, 13, 7542 (2022)
[2] Wührl et al., Phys. Rev. B, 107, 195414 (2023)
[3] Imperor-Clerc et al., Phys. Rev. B, 110, 144106 (2024)

O 6.2 Mon 10:45 H8

**Chromium Oxide Thin Films on Pt(111): An STM and DFT Excursion through the Phase Diagram** — •Ghada Missaoui[1], Piotr Igor Wemhoff[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

Formation of chromium oxide thin films on Pt(111) was investigated by electron diffraction and low-temperature scanning tunneling microscopy. Depending on the nominal Cr coverage and the oxygen-chemical potential used for preparation, two oxide phases were identified. A $(\sqrt{3} \times \sqrt{3})$R30° phase emerges at sub-monolayer Cr exposure and O-rich oxidation conditions, while a (2x2) phase develops at higher coverage and after a vacuum-annealing step. For both phases, the atomic nature of cationic and anionic sub-lattices and the chemical composition were determined in detail. Guided by this experimental input, a global structure optimization was performed by genetic algorithms and key configurations were refined by density functional theory calculations afterwards. For the $(\sqrt{3} \times \sqrt{3})$R30° phase, good agreement was revealed for a $Cr_3O_6$ trilayer, comprising a mixture of $Cr^{3+}$ and $Cr^{4+}$ ions in the central cationic plane. The (2x2) phase matches well a $Cr_6O_{11}$ film, in which an O-Cr-O trilayer is capped by a $Cr_2O_3$ honeycomb plane. The identified configurations not only reproduce structure and symmetry deduced from experiment but also have the most favorable energetics at the employed oxygen chemical potential.

O 6.3 Mon 11:00 H8

**Ferroelectric perovskite oxides: from bulk to surface polarization** — •Dominik Wrana[1], Llorenç Albons[2], Marta Macyk[1], Andrzej Jasicki[1], Aji Alexander[2], Jesus Redondo[2], Igor Sokolovic[3], Pavel Kocan[2], Konrad Szajna[1], Martin Setvin[2], and Franciszek Krok[1] — [1]Institute of Physics, Jagiellonian University, Krakow, Poland — [2]Department of Surface and Plasma Science, Charles University, Prague, Czechia — [3]Institute of Applied Physics, TU Wien, Vienna, Austria

In leveraging the spontaneous polarization of ferroelectrics for photo-, pyro-, and piezocatalysis, it is essential to develop a comprehensive model of ferroelectricity's impact on perovskite surfaces.

Here we investigate oxide perovskites, which are known to exhibit record-high efficiencies toward water spitting. Careful analysis of ferroelectricity exhibited on surfaces of single crystals of as-cleaved ferroelectric $BaTiO_3$(001) and $KNbO_3$(001) compared to quantum paraelectric $KTaO_3$(001) reveals phenomena at both single-atom and macroscales. Polarization optical and scanning electron (SEM) microscopy data provides the spatial information of 90° ferroelectric domains, which typically have a width of 5-20 $\mu$m and length of up to hundreds of um. Actual domain structure and their directionality are provided by piezoresponse force microscopy (PFM) imaging, which also provides the correlation of surface reactivity with polarization.

qPlus ncAFM is used to demonstrate a reversible ferroelectric polarization of (1x1) surfaces at the nanoscale, by application of different tip-sample bias voltages.

O 6.4 Mon 11:15 H8

**The influence of strain-induced ferroelectricity on the fracture of oxide perovskites** — •Christian Ritterhoff and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg

The cleaving of bulk crystals using mechanical force is a common procedure to obtain well-defined surfaces under UHV conditions. While this method avoids chemical changes in the surface composition due to etching and annealing procedures, the strain necessary for cleavage can induce ferroelectric phase transitions during the fracture process whose influence is still visible on the as-cleaved surface, as shown, for example, by Sokolović *et al.* [1] for mechanically cleaved $SrTiO_3$.

Here, we present density-functional theory calculations to discuss the influence of increasing strain on the magnitude of possible ferroelectric distortions and the development of a spontaneous polarization for three prototype perovskite oxides: cubic $SrTiO_3$, ferroelectric $BaTiO_3$, and polar $KTaO_3$. First, we estimate the critical strain for mechanical cleavage in fracture Mode 1 and Mode 2. Subsequently, we calculate the polarization of the material at the point of fracture and discuss the implication on surface charges and the formation of surface defects.

[1] I. Sokolović, M. Schmid, U. Diebold, M. Setvín, Phys. Rev. Mater. **3** (2019) 034407

O 6.5 Mon 11:30 H8

**Segregation Effects in 2D Mixed Oxide Nano-Islands: Edge Structure and Composition in Mixed V-Fe Oxide Monolayers** — Ying Wang[1], Piotr Igor Wemhoff[1], Ghada Missaoui[1], •Niklas Nilius[1], Jacek Goniakowski[2], and Claudine Noguera[2] — [1]Carl von Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne University, UMR 7588, INSP, F-75005 Paris, France

Low-coordinated atoms residing at the edges of oxide nanostructures play an important role in heterogenous catalysis. Their local configuration is however hardly available, especially for ternary materials with variable stoichiometry. In this study, low-temperature STM is employed to analyze the edge configurations of V-Fe-O honeycomb islands grown on Pt(111) as a function of film composition. The islands are delimited by zigzag and armchair edges, the latter with a tendency to reconstruct into sequences of four, five, six and seven-membered rings. STM spectroscopy is used to identify the chemical nature of the edge atoms. The thermodynamic forces for V or Fe segregation to the edges, both oxygen and cation terminated, are analyzed by DFT calculations. In an oxidizing environment, formation of vanadyl-terminated (VO-) edges is energetically favorable, while Fe atoms segregate towards the edges at O-poor conditions. The observed behavior is explained by the higher oxygen affinity of V versus Fe edge cations, and reflected in the higher stability of terminal vanadyl compared to ferryl groups. Our findings indicate a new pathway to tailor the chemical composition and catalytic reactivity of oxide edges via cationic mixing.

O 6.6 Mon 11:45 H8

**Mapping the Energy-Angle-Landscape in lab-based X-ray photoelectron spectroscopy for Depth Profiling of Oxide Layers** — •Martin Wortmann[1,4], Beatrice Bednarz[2], Olga Kuschel[2,3], Klaus Viertel[4], Negin Beryani Nezafat[5], Jan Schmalhorst[1], Gabi Schierning[5], Joachim Wollschläger[3], Andreas Hütten[1], and Timo Kuschel[1,2] — [1]Bielefeld University, Bielefeld, Germany — [2]Johannes Gutenberg University Mainz, Mainz, Germany — [3]University of Osnabrück, Osnabrück, Germany — [4]Bielefeld University of Applied Sciences, Bielefeld, Germany — [5]University of Duisburg-Essen, Duisburg, Germany

Many metals are reactive to atmospheric oxygen, forming stable nanometer-thin oxide layers by spontaneous self-passivation. Such native oxide layers are commonly analyzed by X-ray photoelectron spectroscopy (XPS). We previously introduced a method to calculate depth profiles from single fixed-angle spectra by fitting all emission peaks instead of just one, thus resembling energy-resolved XPS without the need for a synchrotron [1]. Here, we combine this approach with angular-dependent measurements, fitting the measured intensity ratios of oxide and metal as a function of energy (i.e. inelastic mean free path) and angle. This method not only improves the accuracy of earlier models and peak fittings but also paves the way for a more holistic understanding of the XPS spectrum. [1] Wortmann et al., Small Methods 8(3), 2300944 (2024)

O 6.7 Mon 12:00 H8

**The polar spinel $MgAl_2O_4$ (001) surface is stabilized by an aluminum-rich reconstruction** — •David Kugler[1], Andrea Conti[1], Johanna I. Hütner[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 of spinel oxides is key to understanding their catalytic properties. Magnesium aluminate ($MgAl_2O_4$, spinel), which gave this class of materials its name, is a wide-gap insulator and poses considerable challenges for experimental surface structure determination. Noncontact atomic force microscopy (nc-AFM) with a qPlus sensor and a well-defined tip apex allowed us to directly resolve the surface structure with atomic resolution and chemical sensitivity. The $MgAl_2O_4$(001) surface adopts a c(2 × 4) reconstruction accompanied by an increase of the Al/Mg ratio, as detected by x-ray photoelectron spectroscopy (XPS). The reconstructed surface is enriched in aluminum and contains ordered pairs of octahedrally coordinated magnesium atoms replacing their tetrahedral bulk sites. This charge redistribution within the reconstructed surface layer stabilizes the otherwise polar $MgAl_2O_4$(001) termination. The proposed surface reconstruction is similar to those observed on other spinel oxides, such as $Fe_3O_4$(001) and $Mn_3O_4$(001), suggesting a universal mechanism for compensating the polarity of spinel (001) surfaces.

O 6.8 Mon 12:15 H8

**Elucidating the Growth Mechanism of 2D GaS on Sapphire in a Multitechnique Approach** — •Stefan R. Kachel[1,2], Robin Günkel[2], Leonard Neuhaus[1], Oliver Massmeyer[2], Lukas Erlemeier[1], Kassandra Zoltner[1], Florian Münster[1], Carsten von Hänisch[1], Kerstin Volz[2], and J. Michael Gottfried[1] — [1]Department of Chemistry, Philipps-Universität Marburg, Germany — [2]Material Sciences Center and Department of Physics, Philipps-Universität Marburg, Germany

The utilization of 2D layers of GaS with its ultraviolet bandgap holds promise for applications in solar-blind photodiodes and LEDs. However, the growth of these 2D layers remains a significant challenge, driving considerable interest in understanding the growth mechanism underlying the metal-organic chemical vapor deposition (MOCVD) process. This study investigates the growth of 2D GaS using conventional precursors as well as a newly synthesized single-source precursor (SSP) on sapphire in a multitechnique approach. Scanning transmission electron microscopy (STEM) reveals that the formation of a closed Ga layer on the sapphire surface is a prerequisite for GaS growth. This finding is supported by temperature-programmed desorption (TPD) experiments showing intact desorption of the S-precursor, while the Ga-precursor decomposes partially even at low temperatures, leaving Ga residues on the surface, as confirmed by X-ray photoelectron spectroscopy (XPS). The new SSP enables the deposition of thin mixed layers of Ga and S on sapphire. Refining such single-source precursors could provide a pathway toward efficient growth of 2D GaS.

O 6.9 Mon 12:30 H8

**Surface Reconstructions Govern Ice Nucleation on Silver Iodide – A Noncontact-AFM Investigation** — •Johanna I. Hütner[1], Andrea Conti[1], David Kugler[1], Franziska Sabath[3], Florian Mittendorfer[1], Michael Schmid[1], Angelika Kühnle[2], Ulrike Diebold[1], and Jan Balajka[1] — [1]Institute of Applied Physics, TU Wien, Vienna, 1040, Austria — [2]Department of Chemistry, Bielefeld University, Bielefeld, 33615, Germany — [3]Max Planck Institute for Polymer Research, Mainz, 55128, Germany

Silver iodide (AgI) is used as a cloud seeding material due to its ability to nucleate ice efficiently, which is explained by the good lattice match between AgI and hexagonal ice. However, AgI consists of stacked planes of positively charged $Ag^+$ alternating with negatively charged $I^-$. Cleaving a AgI crystal along the (0001) plane thus exposes $Ag^+$ and $I^-$ terminated surfaces. Both terminations are polar and inherently unstable.

We present atomically resolved noncontact atomic force microscopy (NC-AFM) images that show how AgI(0001) surfaces compensate for this non-zero electric dipole perpendicular to the surface. Both Ag and I terminated surfaces form reconstructions, whose structure affects their ice nucleating abilities. NC-AFM images of UHV-cleaved surfaces exposed to water vapor reveal that ice forms an epitaxial layer only on the Ag terminated surface, whereas on the I termination ice forms three-dimensional clusters.

These atomic-level observations could enhance our understanding of ice formation processes in the atmosphere.

# O 7: Focus Session Ultrafast Electron Microscopy at the Space-Time Limit I

Shaping functionalities on the nanoscale is one of the most essential challenges in modern condensed matter research. It requires a comprehensive understanding of the complex interplay of the electronic, spin, and lattice degrees of freedom in materials and requires tailoring energy transfer and dissipation pathways on the smallest length and fastest timescales. Recent instrumentation breakthroughs in different varieties of pump-probe ultrafast electron microscopy have opened the way for accessing electronic and structural dynamics at surfaces, interfaces, and nanostructures with down-to-attosecond resolution in time. While ultrafast photoemission electron microscopy techniques provide supreme sensitivity to spin and electron dynamics in real momentum space, bright ultrashort electron pulses in the ultrafast implementation of more traditional electron microscopes can probe optical states, local magnetization, and lattice dynamics with a nanometer spatial resolution.

This focus session highlights recent advances in ultrafast high-resolution electron probing. These include new instrumentation and techniques, excitations from the THz to X-ray regime, and studying novel phenomena and materials systems. At the same time, it will bring together researchers from the different areas of ultrafast condensed matter physics to foster discussions and new collaborations to explore emergent scientific questions in this field.

Organized by
Armin Feist (MPI Göttingen) and Benjamin Stadtmüller (University Augsburg).

Time: Monday 10:30–12:45 Location: H11

O 7.1 Mon 10:30 H11

**Ultrafast Low-Energy Electron Microscopy** — •Johannes Otto[1,2,3], Leon Brauns[1,2], Benjamin Schröder[1,2], and Claus Ropers[1,2,3] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany — [3]Max Planck School of Photonics

Low-Energy Electron Microscopy (LEEM) allows for imaging the first atomic layers of a surface with nanometer resolution by reflecting a low-energy electron beam [1]. This contribution reports on the first implementation and initial results of Ultrafast LEEM. We replaced the electron source of a conventional instrument with a laser-triggered tip-shaped photoemitter enabling imaging with nanometer spatial and picosecond temporal resolution [2]. We show first real-space dynamics including a thermally-induced intensity suppression (transient Debye-Waller effect) and strain-wave propagation. Additionally, we report on stimulated inelastic electron-light scattering (IELS) at beam energies below 100 eV, as recently proposed theoretically [3]. The demonstrated capabilities of the instrument open up new possibilities to investigate a wide range of dynamical phenomena at surfaces.

[1] W. Telieps and E. Bauer, Surface Science 162, 163 (1985).
[2] A. Feist et al., Ultramicroscopy 176, 63 (2017).
[3] A. P. Synanidis et al., Sci. Adv. 10, eadp4096 (2024).

O 7.2 Mon 10:45 H11

**Ultrafast Electron Dynamics in Surface Plasmon Polariton Nanofoci** — •Pascal Dreher, Alexander Neuhaus, Michael Horn-von Hoegen, and Frank Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany

Surface plasmon polaritons (SPPs) are collective wave-like excitations of the electron system of a metal surface that hold great potential for enhancing light-based energy conversion processes. Such enhancement is based on the efficient generation of highly-excited hot electrons via the decay of SPPs on a femtosecond timescale. To understand the corresponding microscopic dynamics, it is essential to gain a direct view into the plasmonically-generated hot electron distributions and to distinguish them from optically-generated hot electrons.

We achieve these goals by combining topologically-robust SPP nanofoci with time- and angle-resolved photoelectron spectroscopy in a photoemission microscope. This approach allows us to investigate the ultrafast non-equilibrium electron dynamics driven by SPPs on the native length-, momentum-, time-, and energy scales. We observe plasmonically-driven above-threshold electron emission, and ponderomotive shifts of the electron emission spectra provide us with a direct measure of the local SPP field strength. For different exemplary metal surfaces with distinct surface band structures we gain a direct view into the hot electron distributions generated via the coherent and incoherent decay of SPPs.

O 7.3 Mon 11:00 H11

**Mechanisms and Dynamics of Electron Emission from Graphitic Surfaces: Insights from Correlated and Time-Resolved Spectroscopies** — •Alessandra Bellissimo[1], Florian Simperl[1], Felix Blödorn[1], Wolfgang S.M. Werner[1], Gyula Halasi[2], László Óvári[2], Csaba Vass[2], Nikolett Oláh[2], Zoltán Filus[2], Tímea Grósz[2], Chinmoy Biswas[2], Balázs Major[2], Imre Seres[2], Aref Imani[1], Paolo A. Carpeggiani[1], Maosheng Hao[1], and Florian Libisch[1] — [1]TU WIEN, Vienna, Austria — [2]ELI-ALPS, Szeged, Hungary

The electron emission behaviour of graphitic surfaces was investigated using advanced spectroscopic methods alongside static & time-resolved Photo-Electron Emission Microscopy (PEEM). At TU WIEN, electron-pair coincidence spectroscopy on pyrolytic graphite detected *correlated* electron pairs from single scattering events, directly linking energy-loss processes to the secondary electron (SE) spectrum. The $(\pi+\sigma)$-plasmon was resolved in terms of the involved interband transitions revealing strong final-state resonances in the SE spectrum. Static photoemission from graphite(0001) was studied using PEEM at the NanoESCA end station at ELI-ALPS, employing extreme ultraviolet linearly polarised photons generated via High-Harmonic Generation in Argon. The $k$-space-resolved photoelectron (PE) signal associated to the above-mentioned final-state resonances in the SE-spectrum reflects the symmetry of the conduction bands involved in the PE-emission process. Attosecond time- and $k$-space-resolved RABBITT measurements provided insights into PE-emission dynamics across the Brillouin zone.

**Invited Talk** O 7.4 Mon 11:15 H11

**Nanoimaging the electronic, plasmonic, and phononic structure and dynamics of 2D materials** — •Sarah King — University of Chicago, Chicago, IL, United States

Heterogeneity plays a critical role in chemistry and physics, from the role of defect states in the carrier dynamics of semiconductors to interfaces and surfaces in catalysis. However, our ability to visualize nano-scale domains and properties in materials and their effect on material dynamics has been hampered by the simple challenge of our inability to meet the necessary nanometer and femtosecond timescales. I will discuss recent efforts by my group to determine the interplay of heterogeneity and morphology on the intrinsic optoelectronic and thermoelectric properties of materials. Using polarization-dependent photoemission electron microscopy (PD-PEEM) we have imaged the spatially dependent optical selection rules of black phosphorus, distinguishing edge-specific modes, and antiferroelectric domains of $\beta$'-In2Se3, with spatial resolution as good as 25 nm. Through ultrafast transmission electron microscopy, we've been able to determine how the bond anisotropy and structural morphology of few-layer black phosphorus impacts phonon dynamics. Ultimately my group seeks to identify ways to modify the impact of structural heterogeneity in materials and rationally design energy efficient interfaces on the nanoscale.

O 7.5 Mon 11:45 H11

**Time-resolved momentum microscopy with fs-XUV photons at high repetition rates with flexible energy and time resolution** — •Karl Schiller[1], Lasse Sternemann[1], Matija Stupar[1], Alan Omar[2], Martin Hoffmann[2], Jonah Nitschke[1], Valentin Mischke[1], David Janas[1], Stefano Ponzoni[1,3], Giovanni Zamborlini[1,4], Clara Saraceno[2], and Mirko Cinchetti[1] — [1]TU Dortmund University, Dortmund, Germany — [2]Ruhr University Bochum, Germany — [3]Ecole Polytechnique, Paris, France — [4]Karl-Franzens-University Graz, Austria

We present a versatile setup for time-resolved ARPES that combines an energy-filtered momentum microscope with a custom-designed high-harmonic generation (HHG) photon source [1]. The HHG source is powered by a commercial multi-100 kHz Yb-based ultrafast laser system delivering femtosecond pulses in the extreme ultraviolet range. A nonlinear pulse compression stage, utilizing spectral broadening in a Herriott-type bulk multi-pass cell, enables flexible control of the driving pulse duration. This adaptability allows two distinct operational modes, optimized for either energy or time resolution, making the setup highly suitable for ultrafast photoelectron microscopy at the space-time limit. We demonstrate the system's capabilities by tracking conduction band dynamics in the valleys of a bulk $WS_2$ crystal. Using uncompressed laser pulses, we achieve an energy resolution better than $(107 \pm 2)$ meV. Compressed pulses, in contrast, yield a time resolution of $(48.8 \pm 17)$ fs.

[1] Optica Open Preprint 115282 (2024)

O 7.6 Mon 12:00 H11

**Dark field photoelectron momentum microscopy of electric field gated 2D semiconductors** — •Jan Philipp Bange[1], Bent van Wingerden[1], Jonas Pöhls[1], Wiebke Bennecke[1], Paul Werner[1], David Schmitt[1], AbdulAziz AlMutairi[3], Daniel Steil[1], R. Thomas Weitz[1], G. S. Matthijs Jansen[1], Stephan Hofmann[3], Giuseppe Meneghini[2], Samuel Brem[2], Ermin Malic[2], Marcel Reutzel[1], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, Germany — [2]Philipps-Universität Marburg, Germany — [3]University of Cambridge, U.K.

A possibility to tune many-body interactions in two-dimensional semiconductors is in-situ electric field gating, which allows precise and reversible control of the filling of states in a moiré potential. In combination with ARPES for static band structure measurements, this approach has been shown to be a powerful experimental probe [1]. However, the study of excited states in gated 2D material structures, such as interlayer excitons [2] and trions, has so far remained elusive.

Here we combine time-resolved momentum microscopy with dark field imaging techniques to gain access to many-body interactions on femtosecond time and nanometer lengthscales [3]. We use this method to study electric field gated homobilayer $WSe_2$ and report the ultrafast formation of quasiparticles as a function of applied gate voltage.

[1] Nguyen *et al.*, Nature **572**, 220 (2019).
[2] Bange *et al.*, Science Advances **10**, eadi1323 (2024).
[3] Schmitt *et al.*, Nature Photonics, in press, arXiv.2305.18908.

O 7.7 Mon 12:15 H11

**Plasmonic spin meron pair: Spatio-temporal topology revealed by time resolved polarimetric photo-emission microscopy** — Pascal Dreher[1], •Alexander Neuhaus[1], David Janoschka[1], Alexandra Roedl[1], Tim Meiler[2], Bettina Frank[2], Timothy J. Davis[1,2,3], Harald Giessen[2], 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 and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [3]School of Physics, University of Melbourne, Parkville Victoria 3010, Australia

We have developed a novel method, polarimetric photo-emission electron microscopy (polarimetric PEEM), which combines an optical pump-probe polarimetry with photo-emission electron microscopy. This method enables the accurate generation and measurement of surface plasmon polariton fields at deep sub-wavelength spatial resolution and sub-cycle temporal resolution. Using polarimetric PEEM, we extend the study of electromagnetic fields on surfaces to a spin quasiparticle with the topology of a meron pair and analyze its topology by calculating the Chern number. We find the Chern number to be C=1 and constant over time, demonstrating the stability of the plasmonic meron pair on a femtosecond time scale. Additionally, we show that the in-plane vectors of the three-dimensional field are constrained by the embedding topology of the space as dictated by the Poincare-Hopf theorem.

O 7.8 Mon 12:30 H11

**Momentum microscopy with attosecond time resolution at ELI ALPS to map the full Brillouin zone** — Gyula Halasi[1], Csaba Vass[1], Nikolett Oláh[1], Zoltán Filus[1], Tímea Grósz[1], Chinmoy Biswas[1], Tamás Csizmadia[1], Lénárd Gulyás Oldal[1], Balázs Major[1], Péter Jójárt[1], Felix Blödorn[2], Florian Simperl[2], Aref Imani[2], Paolo Carpeggiani[2], Péter Dombi[1], Wolfgang S.M. Werner[2], Alessandra Bellissimo[2], and •László Óvári[1] — [1]ELI ALPS, Szeged, Hungary — [2]Vienna University of Technology, Austria

Time-resolved photoemission is a highly efficient tool for unraveling surface electron dynamics. The coupling of a photoemission electron microscope (PEEM) with an imaging hemispherical analyzer in our NanoESCA end station allows for the combination of spectroscopy and microscopy in real or momentum space. The NanoESCA end station is attached to a high harmonic generation (HHG) beamline, hence time-resolved momentum microscopy studies can be performed in a pump-probe scheme. To illustrate the performance of our user-ready system, the first results obtained by the RABBITT (Reconstruction of Attosecond Beating By Interference of Two-photon Transitions) scheme are presented. In this experiment, a graphite(0001) single crystal was studied, and RABBITT oscillations have been identified throughout the whole Brillouin zone, with attosecond precision, in the form of a time-resolved momentum space movie.

# O 8: Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation I

This focus session aims to discuss recent advances in the on-surface synthesis, manipulation, characterization, and understanding of complex molecular architectures on surfaces. The interest in surface-confined molecular nanostructures emerges from their prospective applications in nanoscale (opto-) electronics, spintronics, solar cells, energy storage devices, and other fields. The bottom-up fabrication of surface-supported nanostructures can be based on molecular self-assembly utilizing non-covalent intermolecular interactions, covalent on-surface synthesis, or the direct manipulation of molecules. Molecular self-assembly usually leads to highly ordered nanostructures, controlled by non-covalent interactions, adsorbate-substrate interactions, as well as thermodynamic and kinetic factors. On-surface synthesis by covalent coupling of reactive precursors adsorbed on metallic, semiconducting, or even insulating surfaces has emerged as a powerful method that has opened new possibilities in exploring new routes towards the synthesis of complex low-dimensional nanostructures with unprecedented material properties, often via novel chemical reactions not available in conventional organic chemistry. Finally, the direct manipulation of molecules with the tip of a scanning probe microscope allows for unprecedented chemical transformations or structural modifications, as envisioned by the pioneers of nanotechnology. This focus session is intended to provide a platform for addressing current trends in these closely linked fields from various perspectives in experiment and theory.

Organized by
Sabine Wenzel (University of Marburg) and Christian Wagner (Forschungszentrum Jülich)

Time: Monday 10:30–13:00 Location: H24

**Invited Talk** O 8.1 Mon 10:30 H24

**Chiral reactions at surfaces elucidated by machine learning and enhanced sampling** — Raymond Amador[1], Enrico Trizio[2], Peilin Kang[2], Umberto Raucci[2], Hannah Bertschi[1], Marcella Iannuzzi[3], Jacob Wright[1], Roland Widmer[1], Oliver Gröning[1], Michele Parrinello[2], and •Daniele Passerone[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — [2]Italian Institute of Technology, Genova, Italy — [3]Department of Chemistry, University of Zurich, Switzerland

Experiments performed at the surface of the chiral intermetallic compound PdGa unleash a fascinating surface chemistry phenomenology including regioselectivity and enantioselectivity, in which the energetics is dominated by mid-range dispersive molecular interactions with the substrate. The corresponding modelling of chiral and prochiral adsorption and reactions requires both a high level of electronic structure theory and an appropriate statistical sampling of the reactants, transition state and products ensemble. We show that machine learning potentials based on DFT molecular dynamics trajectories and recently introduced enhanced sampling techniques allow to describe both the thermodynamics and the kinetics of reactions investigated in the laboratories next-door, such as an Orito-like reaction catalysed by PdGa. Moreover, we study a chirality switching of a bianthracene molecule by applying a method introduced by some of us, based on the committor function and the variational principle that it obeys: its minimum uses a self-consistent procedure that starts from information limited to the initial and final states and reveals the transition state ensemble.

O 8.2 Mon 11:00 H24

**On-surface molecular recognition driven by chalcogen bonding** — •Luca Camilli — University of Rome Tor Vergata

The manipulation of organic architectures on surfaces through supramolecular interactions has been achieved by using, for example, H- and halogen-bonding. Chalcogen bonding interactions (ChBIs), which belongs to the same category, have not. The interest in ChBIs relies on its orbital mixing nature that provides semiconducting properties to the assemblies.[1] Here, we combine scanning tunnelling microscopy measurements and quantum chemistry calculations to present the first example of ChBI-driven molecular self-assembly on metal surfaces.[2] We show that pyrene-based modules bearing chalcogenazole pyridine moieties undergo self-assembly into dimers through double Ch***N interactions on Au(111) and Ag(110). Synchrotron-based spectroscopy techniques are used to gain more insights into the chemistry of the ChBI and to reveal its fingerprint [unpublished data]. Finally, experimental scanning tunnelling spectroscopy and its simulations based on the framework of density functional theory are used to investigate the electronic properties of the self-assembled systems [unpublished data]. This study sheds light on a promising avenue for future research in the bottom-up engineering of two-dimensional monolayered supramolecular chalcogenide-type materials, as we delve into the novel role of ChBIs in surface-based molecular recognition.

References 1. D. Romito et al. Angew. Chem. Int. Ed. 2022, 61 (38), e202202137. 2. L. Camilli, et al. JACS Au 4, 2115 (2024)

O 8.3 Mon 11:15 H24

**Self-assembly, electronic structure, and switching of norbornadiene derivative photoswitches** — •Shreya Garg[1], Vishakya Jayalatharachchi[1], Pedro Ferreira[2], Roberto Robles[3], Sajjan Mohammad[1], Shivani Singh[1], Nicolás Lorente[3,4], Kasper Moth-Poulsen[2], Meike Stöhr[1,5], and Sabine Maier[1] — [1]Department of Physics, Friedrich Alexander University Erlangen-Nürnberg, Germany — [2]Polytechnic University of Catalonia, Catalonia, Spain — [3]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastian, Spain — [4]Donostia International Physics Center (DIPC), San Sebastian — [5]University of Applied Sciences of the Grisons, Switzerland

Molecular photoswitches such as norbornadiene (NBD) derivatives are promising energy storage compounds due to their ability to switch to the metastable quadricyclane (QC) isomer with long half-lives and high-energy storage density. However, the NBD/QC derivative photoswitches remain largely unexplored on the surface. Here, we discuss the self-assembly, electronic structure, and switching of carboxylic acid-functionalized NBD derivative on the Au(111) surface using scanning tunneling microscopy complemented by density functional theory calculations. To explore the impact of the molecule-surface interactions, we also studied them on graphene, which acts as a decoupling layer. We observed distinct hydrogen-bonding motifs between the NBD derivatives on the two surfaces. Our study highlights differences in the electronic properties between the Au(111) and graphene surface, providing insights into optimizing their switching performance on surfaces.

O 8.4 Mon 11:30 H24

**Kinetics of the on-surface reactions of 3,3"-dibromo-p-terphenyl on Cu(111): Cis-trans isomerization as rate limiting step towards the final configurations** — •Mohit Jain[1], Tamam Bohamud[1], Daniel Kohrs[2], Nathaniel Ukah[2], Hermann A. Wegner[2], and Michael Dürr[1] — [1]Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Institut für Organische Chemie and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany

The kinetics of the on-surface synthesis reactions of 3,3"-dibromo-p-terphenyl were investigated at fixed surface temperature of 300 K. The initially adsorbed molecules linked through C-Cu-C bonds were found in configurations consisting of long, chain-like and few shorter ring-like structures. With the progression of the reaction through time at

300 K, the configurations showed a shift from long chains and closed structures to 3-molecule ring structures. These structures then slowly aligned to form surface-wide phases of 3-molecule closed-ring structures.

The lateral surface mobility of the molecules was observed to be high at 300 K along with the frequent cleavage and re-formation of the C-Cu-C bond; nevertheless the actual transformation of chain structures towards complete ring structures was detected at a much longer timescale. By quantitative analysis, the trans-to-cis isomerization of the molecules which is necessary for closed-ring formation, was found to be the rate limiting step. To further consolidate the results, experiments with different substitution patterns of the p-terphenyl molecules were performed.

O 8.5 Mon 11:45 H24

**Stability and Reactivity of Fe-DCA 2D Metal-Organic Framework on Graphene** — •Zdeněk Jakub[1], Dominik Hrůza[1], Taduáš Lesovský[1], Ayesha Jabeen[1], Jakub Planer[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 or 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 a weakly-interacting substrate, graphene/Ir(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 responds to exposure to CO, $O_2$, and thermal annealing. Our data indicate that CO readily adsorbs at room temperature, and the 2D MOF remains stable. In contrast, adsorption of $O_2$ causes structural collapse of the 2D MOF, leaching the Fe cations from the Fe-DCA islands and leaving patches of self-assembled DCA on the surface. Thermally, the Fe-DCA structure decomposes upon annealing above 100 °C. Overall, our work addresses the limits of thermal and chemical stability of metal-DCA systems; such knowledge is relevant for any potential application of these materials.

O 8.6 Mon 12:00 H24

**Tuning the properties of 2D Metal-Organic Frameworks by doping of the support** — •Ayesha Jabeen[1], Zdeněk Jakub[1], Dominik Hrůza[1], Lenka Černá[1], Pavel Procházka[1], Jakub Planer[1], and Jan Čechal[1,2] — [1]CEITEC-Central European Institute of Technology, Brno University of Technology, Purkyňova 123, Brno 61200, Czech Republic — [2]Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2, Brno 61200,Czech Republic

2D metal-organic frameworks (MOFs) are extensively studied due to their tailorable properties, which make them promising for applications in catalysis, energy storage and sensing. Here, we show how the properties of 2D MOFs can be further tuned by varying the energy-level alignment with the supporting surface. We demonstrate this on the case of Ni-TCNQ 2D MOF, that we synthesized atop graphene/Ir(111) with different doping levels. The graphene doping is achieved by intercalation of heteroatoms at the graphene/Ir(111) interface; namely oxygen (for p-doping) and dysprosium (for n-doping). The changes in the support*s Fermi level position are clearly identified by photoemission techniques (XPS/UPS/ARPES). The Ni-TCNQ 2D MOFs supported on differently doped graphene show distinct properties, as evidenced by STM, XPS and LEEM/LEED. Most notably, XPS suggests that the charge state of the embedded Ni atoms can be controlled, as we observe two distinct components of Ni core levels, whose ratio depends on the support′s doping level. These findings highlight the potential of support doping for tailoring the properties of designer 2D MOFs.

O 8.7 Mon 12:15 H24

**Theoretical Investigation of Dibromopyrene and Iodotriphenylene on Sodium Chloride Coated Copper Substrate** — •Florian Pfeiffer[1], Julian Ernst[1], André Schirmeisen[2], Daniel Ebeling[2], and Simone Sanna[1] — [1]Institute for Theoretical Physics, Justus Liebig University Giessen, Germany — [2]Institute for Applied Physics, Justus Liebig University Giessen, Germany

Organic 2D materials are of great interest for various applications in molecular electronics. Increasingly sophisticated methods of on-surface manipulation via probe tips extend the scope of possible structure modifications to tune the (electronic) properties of such nanostructures.

Halogenated organic precursors such as DBP and IT are the building blocks for the assembly of more complex structures. A sodium chloride bilayer helps to electronically decouple the metallic Cu(111) substrate from adsorbates, increasing mobility and thus simplifying manipulation.

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 scanning tunneling and 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 8.8 Mon 12:30 H24

**On-Surface Design of Highly-Ordered Two-Dimensional Networks Stabilized by Nonmetal Atoms** — •Alisson Ceccatto[1,3], Gustavo Campi[2], Vanessa Carreño[1], Eidsa Ferreira[1], Natalie J. Waleska-Wellnhofer[3], Eva Marie Freiberger[3], Simon Jaekel[3], Duncan John Mowbray[2], Christian Papp[3,4], Hans-Peter Steinrück[3], and Abner de Siervo[1] — [1]Geb Wataghin Physics Institute - University of Campinas - Campinas/Brazil — [2]School of Physical Sciences and Nanotechnology, Yachay Tech University, 100119 Urcuquí, Ecuador — [3]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany — [4]Angewandte Physikalische Chemie, FU Berlin, Arnimallee 22, 14195 Berlin, Germany

Supramolecular nanoarchitectures have been widely explored to precisely design low-dimensional materials at atomic and molecular levels. Herein, by combining STM measurements and DFT calculations, we report the 2D self-assembled of 1,3,5-tris[4-(pyridin-4-yl)-[1,1-biphenyl])benzene (TPyPPB) molecules on Ag(111) in the presence of Cl adatoms. The adsorption of the TPyPPB molecules on the clean Ag(111) surface forms a porous SAM stabilized by hydrogen bonds. Such packing can be explored as a host-guest material for atom/molecular confinement. However, in the presence of Cl adatoms, the molecular arrangement changes dramatically. The molecular assembly changes its geometry, forming a non-porous SAM stabilized by unconventional H–Cl–H bonds.

O 8.9 Mon 12:45 H24

**On-surface synthesis of drone-shaped oligomers via carbenes** — •Yunjun Cao[1], Joel Mieres-Perez[2], Julien Frederic Rowen[3], Akshay Hemant Raut[3], Paul Schweer[1], Wolfram Sander[3], Elsa Sanchez-Garcia[2], and Karina Morgenstern[1] — [1]Physical Chemistry I, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Lehrstuhl Physikalische Chemie I, NC 5/72, Ruhr-Universität Bochum, 44801, Bochum — [3]Organic Chemistry II, Ruhr-Universität Bochum, D-44801 Bochum, Germany

The development of on-surface synthesis strategies opens opportunities to fabricate sophisticated nanostructures with tailored geometries, symmetries, and other properties. Here, we demonstrate that carbenes can be used as building blocks for fabricating highly branched oligomers with different symmetries on a Ag(111) surface. We synthesize highly symmetric drone-shaped oligomers, which are formed via C=C coupling of two carbenes to create a core, followed by C-H activation of the core with additional carbenes to create branches. Less symmetric drone-shaped oligomers are formed through the cyclodehydrogenation of the highly symmetric oligomers. The products are investigated by scanning tunneling microscopy and supported by ab initio theoretical modeling.

# O 9: Surface Reactions

Time: Monday 10:30–12:30 Location: H25

O 9.1 Mon 10:30 H25

**Co$_2$ reduction by solvated electrons at the NH$_3$/Cu(111) interface.** — •Maya Heine, Lukas Gierster, and Julia Stähler — Humboldt-Universität zu Berlin, Institut für Chemie

Understanding CO$_2$ reactivity is crucial; the amount of CO$_2$ in the atmosphere continues to rise with no imminent peak in fossil emissions in sight [1]. Previously, solvated electrons ($e_s$) have been suggested to activate CO$_2$ , e.g. by forming surface bound $CO_2^-$ radicals [2]. With time-resolved two-photon photoemission and the amorphous NH$_3$/Cu(111) interface, we can study the energetics and dynamics of $e_s$ on femtosecond timescales [3]. Here, the electrons are localised at the surface and their lifetime depends exponentially on NH$_3$ coverage. On an ultrafast timescale, we can now use $e_s$ to decipher the fundamental rate and steps of CO$_2$ activation. We observe a systematic decrease in the $e_s$ lifetime as CO$_2$ is added and conclude that CO$_2$ opens a new decay channel for $e_s$. Further, increases in the work function serve as indicators of possible reactions: electron attachment to CO$_2$ or activated $CO_2^-$ which has a dipole moment. For thick NH$_3$ films we see a much larger work function increase and bleaching of $e_s$. This suggests that the film thickness controls the lifetime of charged reaction intermediates and thus the reaction pathway. Moreover, we show that $e_s$ attachment to CO$_2$ occurs on a 10s of ps timescale.

[1] Friedlingstein et al. **ESDD** (2024)
[2] Hu et al. **Nat. Commun, 14**, 4767 (2023)
[3] Stähler et al. **Chem. Sci. 2, 5**, 907 (2011)

O 9.2 Mon 10:45 H25

**Exploring on hydrogen evolution reaction performance of borophene monolayer** — •Jing Liu and Axel Gross — Institute of Theoretical Chemistry, Ulm University, Oberberghof 7, 89081 Ulm, Germany

Borophene, a unique graphene-like 2D material composed of boron atoms, has gained significant attention due to its exceptional properties [1]. This study investigates its performance in catalyzing the hydrogen evolution reaction (HER). We focus on four distinct borophene configurations: $\alpha$, $\beta 12$, $\gamma 3$, and trigonal structures [2]. Using density functional theory (DFT), we assess the HER performance of pristine monolayers as well as their interaction with an Ag(111) substrate.

The results show that $\alpha$, $\beta 12$, and $\gamma 3$ monolayers possess exceptional HER activity, evidenced by their optimal Gibbs free energy for H-adsorption. However, their performance is markedly suppressed upon interaction with a Ag(111) support, where borophene-support interaction alters the hydrogen binding properties. By contrast, trigonal structure exhibits limited HER activity in both conditions, reflecting structural characteristics unfavorable for HER.

This work highlights the intrinsic catalytic potential of borophene monolayers while emphasizing the critical influence of substrate interactions.

[1] B. Feng, J. Zhang, Q. Zhong, et al. Experimental realization of two-dimensional boron sheets. *Nature Chem.* 8, 563 (2016).
[2] X. Wu, J. Dai, Y. Zhao, et al. Two-Dimensional Boron Monolayer Sheets. *ACS Nano* 6, 7443 (2012).

O 9.3 Mon 11:00 H25

**Realistic Representations of IrO2 Catalyst Surfaces through Extensive Sampling** — •Hao Wan, Hendrik H. Heenen, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Iridium oxides catalyze the oxygen evolution reaction with unparalleled activity and stability, even under harsh acidic conditions. However, this performance is sensitively correlated to strong structural, compositional and morphological changes of the working catalyst. At the atomic level little is presently known about the true active state, aside from the unlikelihood of it being ideal rutile IrO2.

This situation spans a vast configurational space, the extensive sampling of which (e.g. via parallel tempering) would be intractable with predictive-quality first-principles calculations. Training a machine-learning interatomic potential (MLIP) as an efficient surrogate is challenged by an unprecedented diversity of training structures, as even the bulk structure and composition is unknown. To this end, we create a comprehensive training set by first assembling prototype bulk structures for various IrOx stoichiometries from existing databases. In an active learning loop, this set is then augmented through extensive sampling of diverse surface structures created from the prototypes. The resulting trained MLIP identifies hexagonal ring structures on the rutile (110), (100), (111) facets as most stable configurations under operating potential, aligning with experimental indications. Activity evaluations on these structures using established descriptors effectively capture trends consistent with experimental observations.

O 9.4 Mon 11:15 H25

**Hydrogen Atom Scattering from Graphene on Nickel** — •Sophia Tödter, Yvonne Dorenkamp, and Oliver Bünermann — Institute of Physical Chemistry, Georg-August University, Göttingen, Germany

Previously, H atom scattering from graphene grown on a Pt(111) substrate was investigated in detail by our group [1]. Depending on the experimental conditions, two energy loss channels were observed, one quasi-elastic and one strongly inelastic. For a C-H bond to form, the delocalized electronic structure of graphene has to be locally destroyed. This gives rise to an adsorption barrier. If the hydrogen atom cannot cross the barrier, it is elastically reflected. However, if the atom can cross the barrier, it loses a large amount of energy, which can lead to it sticking to the surface [1]. Pt(111) was chosen because it is a weakly interacting substrate. This allows comparison of the experimental data with simulations of H atom scattering from free-standing graphene. Although good qualitative agreement is achieved between experiment and theory, quantitative agreement cannot be achieved because of the non-negligible substrate effect.

To experimentally study the substrate effect we chose Ni(111) as an additional substrate and performed the same experiments. Ni(111) is a strongly interacting substrate and a much larger substrate effect is expected.

[1] H. Jiang et al., Imaging covalent bond formation by H atom scattering from graphene, Science 264, (2019).

O 9.5 Mon 11:30 H25

**On-Surface Photoreactivity via Reactive Intermediates on a Metal Versus an Insulator** — •Iheb Baklouti[1], Julien F. Rowen[2], Dave Austin[3], Lilian N. Alsayed[1], Talat S. Rahman[3], Wolfram Sander[2], and Karina Morgenstern[1] — [1]Ruhr-Universität Bochum, Chair of Physical Chemistry I, Bochum, Germany — [2]Ruhr-Universität Bochum, Chair of Organic Chemistry II, Bochum, Germany — [3]University of Central Florida, Department of Physics, Orlando, FL, USA

Organic azides play a pivotal role in click chemistry, serving as versatile precursors in synthesizing complex molecules across synthetic chemistry, pharmacology, materials science, and catalysis. Despite their importance, investigations into the surface reactivity of azides remain sparse. This study elucidates the behavior of 2-azidofluorene (2AF) on two distinct surfaces: metallic Ag(100) and ionic NaBr(100), under cryogenic conditions (7 K). Utilizing Infrared Reflection Absorption Spectroscopy (IRRAS) and Scanning Tunneling Microscopy (STM), reactions initiated by ultraviolet illumination are analyzed. Nitrene formation from 2AF is hindered by charge transfer interactions with Ag(100), emphasizing the need for low-interaction surfaces like NaBr(100). Illumination at 254 nm induces 2AF dissociation, forming 2-fluorenylnitrene. Subsequent exposure to 450 nm light leads to didehydroazepines, a process reversible under 405 nm. This study sheds light on azide surface-mediated dynamics and introduces a framework for investigating reactive intermediates in surface chemistry.

O 9.6 Mon 11:45 H25

**Sustainable argon irradiated MWNT-based filters for efficient remediation of methylene blue dye from wastewater: characterization and mechanism** — •Emad Elsehly — Physics Department, Faculty of Science, Damanhour University, 22516, Damanhour, Egypt

This study handles the irradiation of the multi-walled carbon nanotubes by argon ion beam and their potential application for dye removal from wastewater. The obtained data revealed that Argon ion irradiation can induce various structural changes and defects in MWNTs as confirmed by Raman spectroscopy. Moreover, the structural integrity of R-MWNTs is preserved during irradiation as shown by SEM. R-MWNTs yielded smaller crystallites, reaching a size of 4.4 nm. The adsorption efficiency of R-MWNTs was examined by remediation of methylene blue (MB) from wastewater. The results demonstrated that the remediation percentage of R-MWNTs enhanced and could reach 98%. The adsorption mechanism of methylene blue onto R-MWNTs is spontaneous, and almost chemical adsorption process. R-MWNTs have greater surface area and more active sites for adsorption. The irradiation tool offers an alternative approach to enhance the structure of MWNTs-based filters and present a highly effective solution for the removal of dyes from wastewater.

O 9.7 Mon 12:00 H25

**On-surface Synthesis of Non-Benzenoid Nanographenes Embedding Azulene and Stone-Wales Topologies** — •Qifan Chen[1], Kalyan Biswas[2], Sebastian Obermann[3], Ji Ma[3], Diego Soler-Polo[1], Jason Melidonie[3], Ana Barragán[2], Ana Sánchez-Grande[1], Koen Lauwaet[2], Rodolfo Miranda[2], David Écija[2], Pavel Jelínek[1], Xinliang Feng[3], and José Urgel[2] — [1]Institute of Physics of the Czech Academy of Science, CZ-16253 Praha, Czech Republic — [2]IMDEA Nanoscience, C/Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain — [3]Center for Advancing Electronics Dresden & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, D-01069 Dresden, Germany

The incorporation of non-benzenoid motifs in graphene nanostructures significantly impacts their properties. Understanding of the specific reaction mechanism of forming non-benzenoid nanographene structures with tailored electronic/magnetic properties remains limited. In this work, we report a theoretical study addressing an on-surface synthetic strategy toward fabricating non-benzenoid nanographenes containing different combinations of pentagonal and heptagonal rings. We employ the Quantum Mechanics/Molecular Mechanics (QM/MM) approach to analyze the optimal reaction pathways on Au(111) surface and explore the roles of an adatom on the activation energy barrier of the reaction. Our work provides atomistic insight into the reaction mechanism of single gold atom-assisted synthesis of novel NGs containing nonbenzenoid motifs.

O 9.8 Mon 12:15 H25

**Enhanced Sampling of Chiral Molecules on Chiral PdGa Surfaces Using Machine Learning** — •Raymond Christopher Amador[1,2], Umberto Raucci[3], Peilin Kang[3], Enrico Trizio[3], Hannah Bertschi[4], Jacob Wright[2], and Daniele Passerone[1,2] — [1]nanotech@surfaces laboratory, Empa, Zürich, Switzerland — [2]ETH Zürich, Zürich, Switzerland — [3]Italian Institute of Technology, Genova, Italy — [4]Max Planck Institute, Hamburg, Germany

The interaction of chiral molecules with chiral surfaces plays a fundamental role in enantioselective catalysis and molecular recognition processes. In this work, we present a novel machine learning-assisted framework for enhanced sampling of chiral molecule dynamics on chiral PdGa surfaces. Using high-dimensional descriptors of molecular-surface interactions and leveraging state-of-the-art neural network potentials, our approach significantly accelerates the exploration of configurational space while maintaining chemical accuracy. Detailed analysis reveals how chiral PdGa surfaces influence molecular adsorption, orientation, and reaction pathways, providing new insights into the enantioselective mechanisms. These findings demonstrate the potential of integrating machine learning techniques with surface science to address challenges in heterogeneous catalysis.

## O 10: Focus Session Ultrafast Electron Microscopy at the Space-Time Limit II

Shaping functionalities on the nanoscale is one of the most essential challenges in modern condensed matter research. It requires a comprehensive understanding of the complex interplay of the electronic, spin, and lattice degrees of freedom in materials and requires tailoring energy transfer and dissipation pathways on the smallest length and fastest timescales. Recent instrumentation breakthroughs in different varieties of pump-probe ultrafast electron microscopy have opened the way for accessing electronic and structural dynamics at surfaces, interfaces, and nanostructures with down-to-attosecond resolution in time. While ultrafast photoemission electron microscopy techniques provide supreme sensitivity to spin and electron dynamics in real momentum space, bright ultrashort electron pulses in the ultrafast implementation of more traditional electron microscopes can probe optical states, local magnetization, and lattice dynamics with a nanometer spatial resolution.

This focus session highlights recent advances in ultrafast high-resolution electron probing. These include new instrumentation and techniques, excitations from the THz to X-ray regime, and studying novel phenomena and materials systems. At the same time, it will bring together researchers from the different areas of ultrafast condensed matter physics to foster discussions and new collaborations to explore emergent scientific questions in this field.

Organized by
Armin Feist (MPI Göttingen) and Benjamin Stadtmüller (University Augsburg).

Time: Monday 15:00–17:45 Location: H2

**Invited Talk** O 10.1 Mon 15:00 H2

**Probing coherent optical emission processes with ultrafast scanning electron microscopy** — •Albert Polman — NWO Institute AMOLF, Amsterdam, the Netherlands

High-energy electron beams are unique probes of optical materials properties as their time-varying electric field can create strong materials polarizations. The subsequent light emission (cathodoluminescence, CL) provides a fingerprint of the local optical density of states at the nanoscale.

CL from plasmonic and dielectric nanostructures has a coherent phase relation with the excitation process, which enables self-referenced measurements to perform holography and metrology. Electron excitation of semiconductors creates a sequence of fs-ps-ns materials excitations, that lead to bunched CL photon emission.

New developments in ultrafast electron microscopy enable the creation of picosecond electron pulses and pump-probe spectroscopy where light and electrons serve as pump and probe or vice versa. The interaction of pulsed electrons with optical metasurfaces enables novel ways to shape the quantum mechanical electron wavepackets in space and time and may eventually create entirely new forms of ultrafast materials spectroscopy.

O 10.2 Mon 15:30 H2

**Spectrally resolved free electron-light coupling strength in a transition metal dichalcogenide** — •Soufiane El kabil[1], David Lerchenberger[1], Niklas Müller[1], Jonathan Weber[1], Alexander Schröder[1], and Sascha Schäfer[1,2] — [1]University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy, Regensburg, Germany

In ultrafast transmission electron microscopy (UTEM), combining precisely controlled free-electron beams with localized light fields enables the creation of intricate electronic states and the visualization of transient optical near-fields via PINEM [B. Barwick, et al. Nature 462.7275 (2009): 902-906]. However, optical nearfields in photonic structures typically exhibit a strong wavelength dependence, which has so far only been partially captured by PINEM approaches.

To address this, we use strongly chirped broadband light pulses to explore the spectrally resolved interaction between free electrons and light at the edge of a MoS2 thin film [N. Müller, et al. arXiv preprint arXiv:2405.12017(2024).]. As a fast electron traverses the optical field near the MoS2 flake, it absorbs or emits multiple photons, producing photon sidebands in its energy spectrum. By varying the electron-light delay at the sample, different spectral components of the near-field can be investigated. Numerical simulations reveal that the observed spectral and spatial modulations stem from interactions between incident and reflected light fields, as well as guided thin-film optical modes. Our results highlight the ability of PINEM to resolve the optical properties of semiconductors spatially and spectrally.

O 10.3 Mon 15:45 H2

**Simulating Quantum Spin Dynamics in Transmission Electron Microscopy** — •Santiago Beltrán Romero[1,2], Dennis Rätzel[3], Stefan Löffler[2], and Philipp Haslinger[1,2] — [1]VCQ, Atominstitut, TU Wien, Stadionallee 2, 1020 Vienna, Austria — [2]University Service Centre for Transmission Electron Microscopy,TU Wien, Wiedner Hauptstraße 8-10/E057-02, 1040 Wien, Austria — [3]ZARM, Unversität Bremen, Am Fallturm 2, 28359 Bremen, Germany

Transmission Electron Microscopy (TEM) has revolutionized nanoscale research by enabling unprecedented simultaneous spatial and temporal resolutions, thanks to advancements such as aberration correction, cryogenic techniques, and ultra-fast probing. However, the capabilities of TEM to probe spin dynamics – critical for understanding quantum materials – are, to date, quite limited and could be significantly improved by novel microwave spectroscopic tools [1, 2]. Building on recent innovations in that direction, we present a framework that integrates scattering theory and multislice simulations to describe the probing of spin samples on the nanoscale with time-resolved TEM. Our simulations offer insights into both elastic and inelastic processes - including the electrons backaction on the spin. They reveal how the choice of set-up parameters influence the precision of spin detection, identifying optimized conditions for enhancing the signal-to-noise ratio (SNR) and contrast. This work sets the stage for combining spin resonance tools with cutting-edge TEM capabilities, paving the way for breakthroughs in spin imaging and manipulation at the atomic level.

O 10.4 Mon 16:00 H2

**Ultra-Nonlinear Subcycle Photoemission of Few-Electron States from Sharp Gold Nanotapers** — •Germann Hergert, Rasmus Lampe, Andreas Wöste, and Christoph Lienau — Institut für Physik, Carl-von-Ossietzky Universität, 26129 Oldenburg, Germany

Generating attosecond electron pulse trains by coherent modulation of swift electrons enabled attosecond resolution in ultrafast transmission electron microscopy [1,2]. The possibility to transfer photon statistics to the electron number statistics in multiphoton photoemission (MPP) from nanotapers [3], opens up a window to increase photoemission nonlinearities of few-electron states and generating subcycle electron pulses. This provides an alternative road to reach subcycle resolution in electron microscopy.

Here, we present MPP of few-electron wavepackets triggered by near-infrared pulses from gold nanotapers, demonstrating 20th-order nonlinearities for electron triplets. Event-based interferometric autocorrelations of the photoemission yield are quenched to single-peak traces with 0.8 fs duration. We observe a modulation of the electron yield by the carrier-envelope phase, indicating the emission of subcycle isolated electron beams, with prospects to improve the temporal resolution in ultrafast point-projection electron microscopy.

[1] D. Nabben, Nature, 619, 63 (2023)
[2] J. Gaida, Nat. Photon., 18, 509 (2024)
[3] J. Heimerl, Nat. Phys., 20, 945 (2024)
[4] G. Hergert, Nano Lett., 24, 11067 (2024)

**Invited Talk** O 10.5 Mon 16:15 H2

**Ultrafast exciton dynamics in momentum space** — Alexander Neef[1], Tommaso Pincelli[1,2], Lawson Lloyd[1], Shuo Dong[1], Samuel Beaulieu[1], Tania Mukherjee[1,2], Sebastian Hammer[3], Malte Selig[2], Dominik Christiansen[2], Andreas Knorr[2], Martin Wolf[1], Jens Pflaum[3], Laurenz Rettig[1], and •Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Technische Universität Berlin, 10623 Berlin, Germany — [3]Julius-Maximilian-Universität Würzburg, 97070 Würzburg, Germany

Time- and angle-resolved photoemission spectroscopy (trARPES) provides a quantum-state-resolved picture of the ultrafast dynamics of many-body states like excitons in non-equilibrium states of matter. Following the formation and scattering of excitons in momentum space in real time reveals all key properties of the excitons like binding energy, exciton-phonon coupling, and the real-space distribution of the many-body wave functions. Additionally, information about the orbital properties and Berry curvature is encoded in the multidimensional trARPES signals. Applied to heterostructures, the ultrafast exciton and charge dynamics across interfaces reveal the mechanism of charge and energy transfer processes. We will exemplify this approach for transition metal dichalcogenides heterostructures, molecular crystals, and layered semiconducting antiferromagnets.
References: S. Dong et al., Nature Commu. 14, 5057 (2023); T. Pincelli et al., Adv. Mater. 2209100 (2023), A. Neef et al., Nature 616, 275 (2023), S. Beaulieu et al., Sci. Adv. 10, eadk3897 (2024).

O 10.6 Mon 16:45 H2

**Subcycle band-structure videography of quantum materials** — •Vincent Eggers[1], Manuel Meierhofer[1], Jakob Helml[1], Lasse Münster[1], Robert Wallauer[2], Giacomo Inzani[1], Sarah Zajusch[2], Suguru Ito[2], Leon Machtl[1], Yin Hao[3], François C. Posseik[3], Changhua Bao[1], Jens Güdde[2], F. Stefan Tautz[3], Rupert Huber[1], and Ulrich Höfer[1,2] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, Philipps-Universität Marburg, 35037 Marburg, Germany — [3]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany

We introduce the next generation of subcycle band-structure videography. By combining atomically strong few-cycle mid-infrared lightfields with sub-10-femtosecond XUV pulses in a momentum microscope, lightwave-driven dynamics can now be investigated throughout the entire Brillouin zone. Here, we observe electrons driven by carrier fields of light reaching amplitudes as high as MV/cm in graphene. Subcylce analysis of the timing of these lightwave-driven currents reveals femtosecond scattering times. Our novel setup provides a new platform to explore strong-field phenomena ranging from inter- and intraband dynamics to Bloch oscillations and the emergence of Floquet-Bloch states directly in subcycle videos covering the full band structure.

O 10.7 Mon 17:00 H2

**Approaching Atomic Resolution in Ultrafast Transmission Electron Microscopy** — •Sophie Schaible[1,2], Till Domröse[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) [1] extends the study of structural heterogeneity in conventional TEM by introducing femtosecond temporal resolution, providing the means to map structural phase transitions at the nanoscale. However, access to atomic-scale ultrafast dynamics remains a major challenge due to the limited brightness of pulsed photoelectron beams. In this contribution, we explore approaches to atomic-resolution imaging of a structural transformation in a UTEM employing a high-coherence photoelectron source. Highly dose-efficient imaging is crucial to make optimum use of the available electron signal. We further gauge the impact of experimental parameters on the achievable spatiotemporal resolution such as sample drift, acquisition time, repetition rate and electron pulse length with and without optical excitation of the specimen.

[1] Feist *et al.* Ultramicroscopy **176** (2017)

O 10.8 Mon 17:15 H2

**Towards Detection of Spin Resonance Excitations with TEM** — •Antonín Jaroš, Johann Toyfl, Benjamin Czasch, Michael Stanislaus Seifner, Isobel Claire Bicket, Santiago Belrán-Romero, and Philipp Haslinger — VCQ, Atominstitut, TU Wien, USTEM, Stadionallee 2, 1020 Vienna, Austria

Microwave (MW) excitations of spin systems induce precessional spin motion at GHz frequencies. Traditional spin resonance spectroscopy techniques, such as Electron Spin Resonance (ESR) and Ferromagnetic Resonance (FMR), are employed to determine key parameters like gyromagnetic ratios and damping constants in magnetic materials. However, these methods often lack the spin sensitivity and spatial resolution required for spin studies at the atomic level. We present a novel approach that synergistically combines spin resonance techniques with Transmission Electron Microscopy (TEM). Spin state polarization is induced by the magnetic field of the TEM pole piece, while spin system excitation is achieved through an impedance-matched micro-resonator integrated into a custom-designed sample holder. The detection of spin resonance excitations in TEM might represent an important step towards MW driven spin studies with highly controlled electron probe at the nanoscale.

O 10.9 Mon 17:30 H2

**Laser-driven cold-field emission source for ultrafast transmission electron microscopy** — Alexander Schröder[1], •Andreas Wendeln[1,2], Jonathan Weber[1,2], Masaki Mukai[3], Yuji Kohno[3], and Sascha Schäfer[1,4] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Insitute of Physics, Carl-von-Ossietzky Universität Oldenburg, Oldenburg, Germany — [3]JEOL Ltd., Tokio, Japan — [4]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

In recent years ultrafast transmission electron microscopy (UTEM), which combines the nanometer spatial resolution of a TEM with the femtosecond temporal resolution of a pump-probe approach, has become an increasingly important tool for investigating nanoscale dynamics. Further improving the spatio-temporal resolution in time-resolved electron imaging experiments requires femtosecond photoelectron sources with a higher degree-of-coherence. Here, we present the development of a laser-driven cold field electron source integrated in a UTEM instrument [1]. This approach yields 220-fs electron pulses with electron energy widths down to 360 meV, photoelectron spot sizes of 2 Å, and a peak normalized beam brightness exceeding $6.5 \cdot 10^{13}$ A/m$^2$sr, providing a new level of spatial and spectral precision in observing ultrafast nanoscale dynamics for UTEM applications. Lastly, we discuss the implementation of laser-driven cold-field emitters in a probe-aberration-corrected electron microscope potentially leading to smaller spot sizes with less coherent beams and significantly increased electron currents. [1] Schröder et al., arXiv:2410.23961, (2024).

## O 11: Electronic Structure of Surfaces: Spectroscopy, Surface States I

Time: Monday 15:00–18:00 Location: H4

O 11.1 Mon 15:00 H4

**Optimizing the photon detection in inverse photoemission** — •Jan Willermann, Fabian Schöttke, and Markus Donath — Physikalisches Institut, Universität Münster, Münster, Germany

The detection of vacuum-ultraviolet photons ($\hbar\omega = 9.9$ eV) in inverse-photoemission experiments is usually carried out with gas-filled counting tubes. Commonly, iodine/argon gas fillings were used for Geiger-Müller type photon detection. Recently, the gas filling was replaced by acetone to increase stability and the operation was changed to proportional mode [1]. While doing this, the counting tube geometry must not necessarily be changed. We carried out systematic measurements to understand the photon detection process in acetone-filled counting tubes and optimize the geometry accordingly. In the range of optimal gas pressures, we found that the photon mean free path in acetone is in scale of a few millimeters instead of a few centimeters as in iodine/argon. Furthermore, we observed that the electron mean free path in proportional-type counting tubes is also reduced to few millimeters. In comparison, the mean free path of electrons in Geiger-Müller-type counting tubes is in the range of the radius of the counting tube. As a consequence, the position of the cathode wire close to the entrance window becomes a critical parameter for the detection efficiency.

[1] C. Thiede *et al.*, Meas. Sci. Technol. **29**, 065901 (2018).

O 11.2 Mon 15:15 H4

**Excitation-Mediated Transport through Nano-scale Josephson Junctions in the Coulomb Blockade Regime** — •Zhengyuan Liu, Sebastian Scherb, Werner M.J. van Weerdenburg, Daniel Wegner, Nadine Hauptmann, and Alexander A. Khajetoorians — IMM, Radboud University Nijmegen, the Netherlands

Josephson junctions (JJs) are essential for superconducting quantum computing and sensing technologies. It has been shown that superconductivity in elemental BCS superconductors, including those typically used for JJs [1], can persist down to the 2D limit. However, the effects of such quantum confinement on both the electronic structure of a JJ and its subsequent transport remains unclear, and fabricating conventional source-drain JJ devices at the nanometer scale is challenging. Here, we use low-temperature scanning tunneling microscopy and spectroscopy to study the electronic structure and transport of model nano-JJ stacks grown on Si(111) surface. We first characterize the quantum well states and superconducting gap of the underlying layer. Then, we explore how both the dielectric and overlying metallic layer affect the electronic and superconducting states. We study the tunneling transport in the Coulomb blockade limit for a number of JJ stacks, revealing that the conductance is dominated by an excitation mediated process. We also discuss the superconducting properties of these stacks, and the potential to detect superconductivity through their charge transport. [1] Werner M. J. van Weerdenburg et al. Sci. Adv. 9, eadf5500 (2023).

O 11.3 Mon 15:30 H4

**Double Photoemission Spectroscopy of $C_{60}$ on $SrTiO_3$ (001) with high efficiency high-order harmonic light source** — •Kathrin Plass[1], Robin Kamrla[1], Frank O. Schumann[2], and Wolf Widdra[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The photoemission spectroscopy is one of the main tools for studying the electronic structure of solids. However, the effects of electron correlation can only be inferred indirectly. In contrast, double photoemission spectroscopy (DPE) enables the direct observation of such phenomena by detecting pairs of correlated photoelectrons ejected following the absorption of a single photon [1].

$C_{60}$ is considered a strongly correlated material, exhibiting a highly structured valence band spectrum. Recently, we discovered orbital-resolved correlation-induced two-electron binding energy shifts in $C_{60}$. In this study, we analyzed DPE data from $C_{60}$ thin films on $SrTiO_3$(001) obtained using a laboratory-based high-order harmonic generation (HHG) light source operating at MHz repetition rates [2]. By boosting the HHG light source to higher photon energies and repetition rates, we are now able to investigate plasmon-assisted double photoemission in $C_{60}$, predicted recently [3].

[1] J. Berakdar et al., Phys. Rev. Lett. **81**, 3535 (1998)
[2] C.-T. Chiang et al., ELSPEC **200**, 15 (2015)
[3] M. Schüler et al., Sci. Rep. **6**, 24396 (2016)

O 11.4 Mon 15:45 H4

**Surface Orbitroscopy: Emergent Phenomena of Orbital Angular Momentum** — •Maximilian Ünzelmann[1], Tim Figgemeier[1], Begmuhammet Geldiyev[1], Hendrik Bentmann[2], and Friedrich Reinert[1] — [1]Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — [2]QuSpin, NTNU Trondheim, Norway

Quantum degrees of freedom in electronic states are a key facet of modern quantum materials. Recently, the orbital angular momentum (OAM) — an orbital analogue of electron spin — has attracted broad attention in condensed matter and surface physics. For instance, orbitronics has been predicted as a promising route towards new functionalities, such as low-dissipation orbital currents or magnetization switching by orbital torques. In this talk, I will present orbital-sensitive angle-resolved photoemission spectroscopy experiments that demonstrate three key features of the OAM: (i) it acts as a central mediator between lattice and spin in spin-orbit-coupled systems, such as Rashba-type surface states [1,2], (ii) it might be associated with orbital currents, and (iii) its momentum texture carries topological information, giving rise to intriguing paradigms like OAM monopoles [3] or momentum-space quantum vortices [4].

[1] M. Ünzelmann *et al.*, Phys. Rev. Lett. **124**, 176401 (2021), [2] B. Geldiyev, M.Ü., *et al.*, Phys. Rev. B **108**, L121107 (2023), [3] M. Ünzelmann *et al.*, Nat. Commun. **12**, 3650 (2021), [4] T. Figgemeier, M.Ü., *et al.*, arXiv:2402.10031 (2024)

O 11.5 Mon 16:00 H4

**Computationally Efficient First-Principles Treatment of Scat-**

**tering States in Photoemission: A Pseudo-potential Approach** — •Gian Parusa[1,2,3] and Michael Schüler[1,2,3] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Paul Scherrer Institute, 5232 Villigen PSI, Switzerland — [3]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland

The calculation of photoemission matrix elements requires the consideration of several key factors, including Bloch states, light-matter coupling, and scattering states. The evaluation of scattering states in solids from first-principles, particularly within a plane-wave basis, is computationally demanding due to the large number of plane waves required at high energies. A well-established strategy for reducing the computational cost in the treatment of valence states involves the use of pseudo-potentials. In this work, we extend the concept of optimized norm-conserving pseudo-potentials to scattering states, utilizing a non-local Vanderbilt projector to restore the wave function properties at a specified target energy. This approach is applied to scattering states, specifically for energies above 1 Rydberg. The method is validated by simulating the photoemission spectrum of graphene and hexagonal boron nitride (h-BN) with the results compared to all-electron calculations, demonstrating both the accuracy and computational efficiency of the proposed technique.

O 11.6 Mon 16:15 H4

**Electronic structure of ferromagnetic CrTe** — •Chien-Wen Chuang[1], Muthu P.T. Masilamani[1], Hibiki Orio[1], Maximilian Ünzelmann[1], Chia-Nung Kuo[2,3], Chin-Shan Lue[2,3], Ashish Chainani[4], and Friedrich Reinert[1] — [1]Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [2]Department of Physics, National Cheng Kung University, Tainan, Taiwan — [3]Taiwan Consortium of Emergent Crystalline Materials, National Science and Technology Council, Taipei, Taiwan — [4]National Synchrotron Radiation Research Center, Hsinchu, Taiwan

Recent studies showed that CrTe and doped CrTe exhibit various emergent properties, such as a large magnetocaloric effect, spontaneous skyrmions and ferromagnetism with high Curie temperature $T_C \sim 340$ K. We carried out Cr L-edge ($2p$-$3d$) X-ray absorption spectroscopy (XAS) and resonant photoemission spectroscopy (Res-PES) with right and left circularly polarized light on single crystal CrTe to investigate the role of Coulomb correlations in Cr $3d$ density of states(DOS). The Res-PES spectra showed a resonantly enhanced sharp peak at a binding energy of 1.5 eV, which corresponds to the Cr main $3d$ DOS, while states at the Fermi level do not show a clear resonance enhancement. A small circular dichroism of Cr $3d$ DOS was observed. In addition, we observed the Cr $3d$ two-hole $L_3VV$ Auger feature which corresponds to a correlation satellite. Using the Cini-Sawatzky method, we estimate the on-site Coulomb interaction energy in Cr $3d$ states to be $U_{dd} \sim 3$ eV.

O 11.7 Mon 16:30 H4

**Unveiling the Role of Inelastic Mean Free Path in Photoelectron Diffraction: A Computational Study by Multiple Scattering** — •Trung-Phuc Vo[1,2], Olena Tkach[3], Sylvain Tricot[4], Didier Sébilleau[4], Aimo Winkelmann[5], Olena Fedchenko[3], Yaryna Lytvynenko[3,6], Dmitry Vasilyev[3], Hans-Joachim Elmers[3], Gerd Schönhense[3], and Ján Minár[1] — [1]Univ. West Bohemia, Czech Republic — [2]Institute of Physics, Czech Academy of Sciences, Czech Republic — [3]Univ. Mainz, Germany — [4]Univ. Rennes, IPR, France — [5]AGH Univ. Krakow, Poland — [6]Institute of Magnetism of the NAS of Ukraine and MES of Ukraine, Ukraine

The inelastic mean free path (IMFP) of electrons near solid surfaces describes the average distance an electron travels through a solid before losing its kinetic energy via inelastic collisions. In surface analysis techniques such as photoelectron diffraction (PED), a short IMFP makes photoelectrons highly surface sensitive, allowing precise structural determination of surfaces. Conversely, a longer IMFP allows access to deeper layers, facilitating the study of bulk properties. The influence of the IMFP on PED is particularly evident with the advent of advanced time-of-flight (ToF) measurements. Controlling this key parameter is crucial. In this work, we summarize the PED implementation within the SPRKKR package and systematically explore its application over a wide kinetic energy range (106-1036 eV) for Ge 3d core levels. Our computational efforts provide insight into both Kikuchi diffraction patterns and their relation to valence band mapping, thus bridging PED analysis with electronic structure studies.

O 11.8 Mon 16:45 H4

**Towards accessing the initial state by dichroic photoemission** — •Jakub Schusser[1,2], Hibiki Orio[1], Maximilian Ünzelmann[1], Johannes Hessdörfer[1], Muthu Prasath Thirugnanasambandam Masilamani Masilamani[1], Florian Diekmann[3,4], Kai Rossnagel[3,4], and Friedrich Reinert[1] — [1]Experimentelle Physik VII and Würzburg- Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [2]University of West Bohemia, Pilsen, Czech Republic — [3]Ruprecht Haensel Laboratory, DESY, Hamburg, Germany — [4]Institute of Experimental and Applied Physics, Kiel University, Germany

Despite its many advantages, photoemission has so far not allowed direct experimental access to detailed information about the initial state of solids. Dichroism in angle-resolved photoemission spectroscopy arises inherently from the matrix-element effects that depend on the initial and final states as well as the light field perturbation. By comparing both experimental and theoretical soft X-ray data in bulk $WSe_2$ we show the robustness of the newly introduced dichroic technique against variation of photon energy, light polarization and angle of incidence. Such robustness of the matrix-element effect represents a leap towards accessing the initial state by this differential technique with high relevance in the field of topological materials, layered systems and other material classes.

O 11.9 Mon 17:00 H4

**Surface electronic structure of Te chains on Au(100) via ARPES** — •Begmuhammet Geldiyev[1], Maximilian Ünzelmann[1], Tim Figgemeier[1], Hendrik Bentmann[2], and Friedrich Reinert[1] — [1]Experimentelle Physik 7 and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [2]Center for Quantum Spintronics, Department of Physics, NTNU, Norway

In this talk, we will provide a comprehensive description of the surface electronic band structure in epitaxial Te chains grown in the submonolayer regime on a Au(100) substrate. First, the deposition of 0.25 ML Te results in an adlayer square lattice superstructure with $p(2 \times 2)$ periodicity. Particularly, the band structure of this system features an interface state – derived from hybrid Te-Au orbitals – that exhibits an anisotropic spin and orbital Rashba effect [1]. Second, by slightly increasing the Te coverage to 0.30 ML, the earlier square arrangement evolves into a chain structure with $c(10 \times 2)$ periodicity [2]. Here, we will address whether the latter system inherits an analogous Rashba effect scenario. Furthermore, we will unravel a flat electronic band with a bandwidth of $\approx 20$ meV, indicating an almost perfect one-dimensional character.

[1] B. Geldiyev et al., Phys. Rev. B 108, L121107 (2023)
[2] L. Hammer et al., Surf. Sci. 750, 122589 (2024)

O 11.10 Mon 17:15 H4

**Unoccupied electronic structure of the AgTe/Ag(111) surface alloy: A spin-resolved inverse photoemission study** — •Marcel Holtmann, Carolin Benfer, and Markus Donath — Physikalisches Institut, Münster University, Germany

The AgTe/Ag(111) surface-alloy system has recently been investigated to understand the microscopic origin of the Rashba effect [1]. ARPES measurements suggest that tellurium $p$ orbitals hybridize with states of the Ag(111) substrate resulting in two $p_{xy}$ valence bands. For the unoccupied band structure, a third hybridization state with out-of-plane symmetry is detected using two-photon photoemission. Apart from this, the unoccupied electronic structure of AgTe/Ag(111) remains unexplored.

We employed spin- and angle-resolved inverse photoemission (IPE) to measure the unoccupied electronic structure with a broader scope. Using our rotatable spin-polarized electron source, we were able to measure the three-dimensional spin texture of the unoccupied states. As expected in [1], we found that the hybridization state shows a large Rashba-type spin splitting, which is untypical for non-heavy-metal systems. Using several photon detectors at different take-off angles to measure the angular distribution of the emitted photons, we gained access to the orbital symmetries of the involved electronic states. In addition, like the pristine Ag(111) surface, the AgTe/Ag(111) surface hosts an image-potential state.

[1] M. Ünzelmann *et al.,* Phys. Rev. Lett. **124**, 176401 (2020)

O 11.11 Mon 17:30 H4

**Surface Sensitivity of the VLEED Scattering Process at Pt(111)** — •Hannah Unterberg, Christoph Angrick, and Markus Donath — Universität Münster, Germany

The diffraction pattern of low-energy electrons (LEED) from Pt(111) shows a three-fold symmetry, although the surface layer exhibits a six-fold symmetry. This result proves the non-neglible influence of the second and deeper atomic layers resulting from the finite probing depth of the electrons. Here, we report on a spin-polarized very-low-energy electron diffraction (VLEED) [1,2] experiment on Pt(111). The reflected specular beam is measured at a fixed polar angle of incidence $\Theta = 45^\circ$, while the azimuthal angle of incidence is varied over a wide range. This allows us to probe the surface sensitivity of the VLEED scattering process.

Our measurements at the non-reconstructed Pt(111) surface reveal distinct differences in the electron reflectivity and the spin-orbit-induced reflection asymmetry along the high symmetry directions $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{M}}$'. These directions are equivalent (non-equivalent) in the case of six (three)-fold rotational symmetry. Our result indicates a substantial contribution from both the first and subsequent atomic layers to the VLEED scattering process. In contrast, results for the Au(111) surface, which hosts the prominent herringbone reconstruction, exhibit only minor differences between $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{M}}$'. The different results for Pt(111) and Au(111) are discussed in view of the reconstruction.

[1] U. Burgbacher *et al.*, Phys. Rev. B **87**, 195411 (2013)
[2] C. Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020)

O 11.12 Mon 17:45 H4

**Broadband THz Non-Linear Response In Topological Noble Metal Dichalcogenides** — George de Coster[1,2], Lucas Lafeta[3], Stefan Heiserer[1], Zdeněk Sofer[4], Achim Hartschuh[3], Georg Duesberg[1], and •Paul Seifert[1] — [1]Institute of Physics, University of the Bundeswehr Munich, EIT, Werner-Heisenberg-Weg. 39, 85577 Neubiberg, Germany — [2]DEVCOM Army Research Laboratory, 2800 Powder Mill Road, Adelphi, Maryland, United States — [3]Department of Chemistry and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Butenandtstraße 5-13 (E), 81377 Munich, Germany — [4]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic

Noble metal dichalcogenides belong to the material class of layered 2D materials and were shown to host type-II Dirac semi-metallic behavior, as well as topological surface states and superconductivity. Intriguingly, noble metal dichalcogenides display strong second harmonic generation and second order photocurrent response despite their centrosymmetric crystal structure. We investigate the spectrally-resolved optical response and reveal second and third order non-linear response at both, optical frequencies as well as in the THz range. The latter is analyzed in polarization resolved spectroscopy, that points towards spin-polarized bands at the symmetry broken surface as origin of the non-linearities. Our results elucidate the spectral opto- electronic response at low energies and discuss its anisotropy in light of underlying symmetry constraints.

## O 12: Nanostructures at Surfaces I

Time: Monday 15:00–17:45 Location: H6

O 12.1 Mon 15:00 H6

**Imaging standing phonons within topological defect in strong coupling superconductor by scanning tunneling microscopy** — •Qili Li, Thomas Gozlinski, Rolf Heid, Jörg Schmalian, and Wulf Wulfhekel — Karlsruhe Institute of Technology, Karlsruhe, Germany

Electron-phonon coupling plays an important role in conventional superconductors. Understanding the behavior of phonons will promote the applications of conventional superconductors. However, it is difficult to observe the spatial behavior of phonons. Here, we utilize inelastic scanning tunneling microscopy (ISTS) at 45 mK to investigate phonons within topological defect, i.e. stacking fault tetrahedron (SFT), in the strong coupling superconductor Pb(111) [1]. We find that the local Eliashberg function [2,3] is significantly enhanced by SFTs. Moreover, lateral standing waves of phonon are also observed on SFTs. Compared with phonon bandstructure, we find that the SFTs have strong confinement on transverse acoustic phonons, while the longitudinal acoustic phonons are less confined. Our findings pave the way to phonon engineering in strong coupling superconductors. [1] PRL 14, 108 (1965). [2] Sov. Phys. JETP 11, 696 (1960). [3] PRL 114, 047002 (2015).

O 12.2 Mon 15:15 H6

**Directing far- and nearfield scattering with dielectric Mie Voids** — •Benjamin Reichel[1], Mario Hentschel[1], Adrià Canós Valero[2], Thomas Weiss[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute of Physics, University of Graz, and NAWI Graz, Graz 8010, Austria

Controlling the behavior of light at the nanoscale is a significant challenge in various applications such as metadevices, diffraction gratings, and resonant surfaces. Recently, Mie voids created in high-index dielectric host materials have emerged as a promising platform for confining electromagnetic waves in small values, possibly extending down to ultraviolet wavelengths in air. Therefore understanding and theoretical modeling the electromagnetic scattering behavior of Mie voids are crucial for their effective use.

In this study, we perform a spectral multipolar decomposition for the far- and near-field scattering behavior of dielectric Mie voids upon plane wave or local point dipole illumination. Dielectric Mie voids exhibit strong forward far-field scattering behavior, whereas in the near-field strong backscattering behavior is observed. These insights will be important in the development of resonance and meta structure designs, especially when deriving a generalized Kerker condition. Finally, leveraging the full resolution of electromagnetic Mie voids will open avenues for embedding quantum emitters in high index substrates.

O 12.3 Mon 15:30 H6

**Influence of Plasma on the Electrode and the Electrolyte during Plasma Electrolysis** — •Lukas Forschner[1], Jan-Luca Gembus[2], Peter Awakowicz[2], Andrew R. Gibson[3], Timo Jacob[1], and Albert K. Engstfeld[1] — [1]Ulm University, Institute of Electrochemistry, Ulm, Germany — [2]Ruhr University Bochum, Chair of Applied Electrodynamics and Plasma Technology, Bochum, Germany — [3]University of York, York Plasma Institute, Heslington, United Kingdom

During plasma electrolysis, a plasma is ignited in a thin vapor layer between the powered electrode and the liquid electrolyte. The plasma interacts with both the electrode[1] and the electrolyte, which can modify their properties.[2] In this work, we focus on a metal electrode used as a cathode, where nanoparticle formation can be observed during plasma electrolysis. To gain fundamental insight into nanoparticle formation, we studied the gas sheath surrounding the electrode (including the plasma) and the respective interfaces in detail. Specifically, we use optical emission spectroscopy and high-speed camera imaging to analyze the processes on a milli- to microsecond time scale. We elucidate the structural changes on the electrode induced by the plasma under these conditions with scanning electron microscopy imaging. Based on these results, we discuss mechanisms leading to the formation of nanoparticles in the solution from the electrode.

[1] Artmann et al., *ChemPhysChem* **22** (2021) 2429.
[2] Forschner et al. *J. Phys. Chem. C* **127** (2023) 4394.

O 12.4 Mon 15:45 H6

**Structural, morphological and chemical characterization of plasma-treated NiCoO electrolyzer anodes** — •Timo Wagner[1], Nicolas Wöhrl[1], Vineetha Vinayakumar[2], Christian Marcks[3], Anna Mechler[3], Doris Segets[2], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]IVG-PST and CENIDE, University of Duisburg-Essen — [3]AVT.ERT, RWTH Aachen University

Plasma surface pre and post treatment are important steps to tailor characteristics for later manufacturing steps, or as a finishing step to engineer surface characteristics for later applications. We developed a nitrogen microwave plasma process to be used as pre and post treatment for NiCoO coatings for electrolyzers. The plasma treatment resulted in significant modification of the NiCoO films. For example a porous structure, as measured by AFM, SEM and TEM, leads to enhanced accessibility of the active material. Organic species from the spray coating were removed and the plasma-treated NiCoO layers also exhibited a highly hydrophilic surface, which facilitated better interaction with the electrolyte. X-ray absorption spectroscopy (XAS) studies indicated a higher Fe uptake from the electrolyte, which is beneficial for the oxygen evolution reaction (OER). Raman studies showed a more reversible oxidation behavior in the plasma-treated layers. Overall, these modifications contributed to an enhanced OER performance of the NiCoO anodes due to the plasma post-treatment as characterized electrochemically by cyclic voltammetry (CV) and measuring the electrochemically active surface area (ECSA).

O 12.5 Mon 16:00 H6

**Artificial Atoms: Energy-Level Engineering and Shape-Dependent Reactivity** — •Marco Weiss, Fabian Stilp, Michael Roessner, Max Reinhart, and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg

Artificially arranged nanostructures can confine the quasi-free two-dimensional electron gas present on noble metal surfaces, giving rise to a series of resonant eigenstates [e.g. 1-3]. These structures, often referred to as artificial atoms, exhibit remarkable parallels to natural atoms, including the ability to form chemical bonds with natural atoms or repulsive interactions with chemically inert molecules. [4] In our previous investigations using atomic force microscopy (AFM), we successfully identified the occupation of resonant eigenstates that intersect the Fermi level. Notably, we observed a probe-tip-induced energy shift of these states during the measurements. [4] Building on these findings, we developed a method to estimate the energy of artificial atomic states based on their electron occupation. This approach enables precise tuning of the energy levels of these states with meV-scale accuracy. Additionally, we discovered that the distance-dependent repulsive interaction between a chemically inert molecule and the resonant eigenstates of the artificial atom is influenced by the geometric shape of the nanostructure. This holds the potential to tailor nanoscale interactions through precise structural design. [1] Crommie et al., Science 262 (1993), [2] Manoharan et al., Nature 403 (2000), [3] Freeney et al., SciPost Phys. 9 (2020), [4] Stilp et al., Science 372 (2021)

O 12.6 Mon 16:15 H6

**Increasing the lifetime of confined electronic states in an artificial quantum structure** — Marco Weiss, •Michael Schelchshorn, Fabian Stilp, Alfred J. Weymouth, and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Understanding and tuning the factors influencing the lifetime of confined electronic states is a basic concept of quantum mechanics, whereas achieving large lifetimes in artificial nanostructures holds great potential for advancing quantum technologies. An example of such artificial structures are CO-based quantum corrals. In this study, tunneling spectroscopy measurements reveal a strong correlation between the size of the quantum corral and spectral width, characterized by a predominant Gaussian line shape. We attribute this dominant Gaussian-shaped lifetime broadening to the interaction of surface state electrons with the corral boundary. To further investigate this phenomenon, we constructed corrals of varying wall densities. Our findings indicate that elastic processes, such as tunneling, are more sensitive to the wall density than coupling to the bulk.

O 12.7 Mon 16:30 H6

**Template-Assisted Synthesis of $Fe_3O_4$ Nanodots for High-Density Resistive Switching Memory** — •Yifan Xu[1,2], Connie Bednarski-Meinke[2], Erkai Wang[3], Asmaa Qdemat[2], Emmanuel Kennzinger[2], Felix Gunkel[3], Regina Dittmann[3], Yen-Po Liu[3], Oleg Petracic[2,1], and Mai Hussein Hamed[2,4] — [1]Heinrich Heine University Düsseldorf, Faculty of Mathematics and Natural Sciences, 40225 Düsseldorf, Germany — [2]Jülich Centre for Neutron Science (JCNS-2), JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Peter Grünberg Institute and JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany — [4]Faculty of Science, Helwan University, 11795 Cairo, Egypt

The growing demand for high-density memory solutions has driven the exploration of innovative fabrication techniques. We introduce a bottom-up approach for synthesizing ordered $Fe_3O_4$ nanodots for nanoscale resistive switching memory applications. Using anodic aluminum oxide (AAO) templates as masks, $Fe_3O_4$ nanodots on Nb:$SrTiO_3$ substrate were fabricated via pulsed laser deposition. Scanning electron microscopy (SEM) confirms the nanodots' uniformity. Grazing incidence X-ray scattering (GISAXS) reveals a high degree of long-range ordering. Magnetometry measurements show that the Verwey transition temperature ($T_V$) and coercivity are preserved compared to continuous thin films. Conductive atomic force microscopy (cAFM) confirms well-defined nanodots using current maps. By sweeping the voltage on a single nanodot, set and reset processes are observed within ±2V.

O 12.8 Mon 16:45 H6

**Intercalation of graphene nanoribbons** — •Lüthi Dominik[1], Lin Yang[2], Ji Ma[2], Akimitsu Narita[3,4], Xinliang Feng[2], Klaus Müllen[3], Pascal Ruffieux[1], Roman Fasel[1], and Gabriela Borin Barin[1] — [1]Empa, Ueberlandstrasse 129, 8600 Dübendorf, Switzerland — [2]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [3]Max Plank Institute for Polymer Research, 55128 Mainz, Germany — [4]Okinawa Institute of Science and Technology, Okinawa 904-0495, Japan

Atomically precise graphene nanoribbons (GNRs) exhibit unique properties due to electron confinement and tunable band gaps, making them ideal for applications ranging from transistors to spintronics. Precise fabrication is critical, and on-surface synthesis enables the creation of various GNR types with tailored edge topologies, giving rise to intriguing properties such as spin-polarized edges and topological quantum states.

For device integration, GNRs must be transferred from metallic to insulating substrates. However, the high chemical reactivity of zigzag edges has hindered studies of their transport properties. To address this, we explore intercalation to decouple GNRs from metallic substrates, enabling dry-transfer in ultra-high vacuum. This preserves intrinsic properties and facilitates integration into device architectures.

We investigate intercalation with transition metal halides, providing a platform to study interactions with magnetic layers, combining decoupling benefits with potential applications in quantum technologies.

O 12.9 Mon 17:00 H6

**Facilitating On-Surface Synthesis on Inert Surfaces by Using a Noble Gas Atmosphere** — •Lukas Grossmann[1], Sascha Korn[2], Rochus Breuer[3], Michael Schmittel[3], Heiko Weber[2], Wolfgang Heckl[1], and Markus Lackinger[1] — [1]Deutsches Museum, Munich, Germany — [2]Friedrich-Alexander University, Erlangen, Germany — [3]University of Siegen, Siegen, Germany

A decisive milestone of On-Surface Synthesis (OSS) is the transition from reactive to inert surfaces for the covalent coupling of molecules. This is desirable, because conventionally used metal surfaces strongly interact with organic adsorbates. Thus, adsorption on metals alters the intrinsic properties of the synthesized nanostructures, compromising their applicability. In contrast, inert surfaces leave the adsorbed nanostructures unperturbed. But synthesis is aggravated since activation energies for coupling reactions on inert surfaces are generally higher than on metals. Consequently, reactants desorb before the activation temperature required for their covalent coupling is reached. Here, we explore the OSS of covalent thioether-linked Sierpinski triangles from 1,3,5-tris(4-mercaptophenyl)benzene on inert graphite surfaces. As shown by Scanning Tunneling Microscopy, covalent coupling is feasible by annealing in an argon atmosphere of 1 bar instead of in a vacuum. This protocol kinetically inhibits the premature desorption of reactants, and could be successfully transferred to even more weakly interacting graphene surfaces. The adsorbed Sierpinski triangles exhibit superior thermal stability compared to identical structures on gold and are air stable, underscoring the advantages of inert surfaces.

O 12.10 Mon 17:15 H6

**Functionalization of Surfaces with Ordered Arrays of Fullerenes** — •Lukas Spree, Caroline Hommel, Pierre Josse, and Andreas Heinrich — IBS Center for Quantum Nanoscience, 52 Ewhayeodae-gil, Daehyeon-dong, 03760 Seoul, South Korea

Endohedral fullerenes are a fascinating class of compounds that facilitate the stabilization of exotic configurations of few-atom structures within the confines of a carbon cage. Depending on the combination of carbon cage and encapsulated species, they provide very stable compounds with highly desirable physical properties. Among the compounds isolated and characterized so far are single molecule magnets with high blocking temperatures and promising candidates for spin qubits with long coherence times.

The exceptional chemical stability of endohedral fullerenes makes them very promising candidates for real-world applications. To achieve their full potential as nanometer sized magnets or quantum sensors, it is necessary to characterize and control the spatial orientation and surrounding of each individual molecule. Scanning probe microscopy techniques lend themselves well for the characterization of ordered assemblies on atomically flat substrates, as they offer an unparalleled combination of spatial and energy resolution.

In this presentation we will show our ongoing efforts of preparing ordered low-dimensional assemblies of endohedral fullerenes on surfaces through chemical functionalization and on-surface synthesis approaches, and discuss possibilities to preserve their desirable properties, like slow magnetic relaxation and potentially long coherence times.

O 12.11 Mon 17:30 H6

**Well-defined nanostructures for energy storage and conversion applications** — •Ningxiang Wu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Template-based technique provides a perfect approach to realize well-defined arrayed nanostructures within large-scale.[1]We have developed nanostructuring techniques mainly using anodic aluminum oxide templates with scalable, parallel and fast processes for fabricating different three-dimensional and surface nanostructures.[2]The obtained well-defined nanostructures possess large-scale arrayed configuration, high structural density, perfect regularity and cost-effectiveness, and are highly desirable for constructing different nano-devices especially for energy storage and conversion applications, including rechargeable sodium-ion and potassium-ion batteries, supercapacitors, and photo electrochemical devices.[3-4]The device performances demonstrated that the obtained nanostructures benefit these applications through the precise control over the structural features enabled by the geometrical characteristics of the templates. These achievements indicate the high potential and importance of template-based nanostructuring techniques for both basic research and device applications.[1] Nat.Commun.,2022,13,2435, [2] Nat.Nanotechnol.,2017,12,244, [3] Nat.Commun.,2018,9,1720, [4] Nat.Commun.,2016,7,10348

## O 13: Organic Molecules on Inorganic Substrates: Adsorption and Growth

Time: Monday 15:00–17:30 Location: H8

O 13.1 Mon 15:00 H8

**Identical Fe-N4 Sites with Different Reactivity: Elucidating the Effect of Support Curvature** — •Dominik Hrůza[1], Zdeněk Jakub[1], Jakub Planer[1], Azin Shahsavar[1], Jiří Pavelec[2], and Jan Čechal[1,3] — [1]CEITEC - Central European Institute of Technology, Brno University of Technology, Czech Republic — [2]Institute of Applied Physics, TU Wien, Vienna, Austria — [3]Faculty of Mechanical Engineering, Brno University of Technology, Czech Republic

Understanding the atomic-scale mechanisms of single-atom catalysts (SACs) is pivotal for advancing their design and application. Using a 2D metal-organic framework (MOF) featuring Fe-N4 sites on a graphene/Ir(111) support, we uncover how the curvature of an inert substrate can significantly influence adsorption properties. We show that a 0.4 Å corrugation induced by the inert graphene/Ir(111) moiré leads to pronounced variations in adsorption energy of TCNQ (tetracyanoquinodimethane) molecules adsorbed on the 2D MOF. Molecules adsorbed above the "valleys" of the graphene/Ir moiré exhibit binding energies significantly stronger than those above the "hills," resulting in a temperature stability difference of over 60 °C. Our findings based on STM and DFT highlight those small structural distortions in SAC structure can profoundly impact the adsorption properties.

O 13.2 Mon 15:15 H8

**Small atoms – large influence: Structural evolution upon dehydrogenation** — •Jonas Brandhoff[1], Alina Preibsch[1], Richard Berger[2], Felix Otto[1], Roman Forker[1], Oliver T. Hofmann[2], and Torsten Fritz[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

Molecular self-assembly is governed by the delicate balance between molecule-substrate and intermolecular interactions. Surface reactions can modulate this balance, enabling the engineering of tailored molecular architectures. Dehydrogenation is one of such surface reactions. Despite hydrogen being often overlooked as the smallest atom, its removal can significantly alter molecular interactions. In this study, 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP) serves as a prototypical molecule to investigate dehydrogenation processes on surfaces. HHTP contains six equivalent hydroxy groups, allowing for varying degrees of dehydrogenation. These can be controlled via variation of the substrate temperature during deposition or using annealing steps post-deposition. Utilizing distortion-corrected Low-Energy Electron Diffraction (LEED), Scanning Tunneling Microscopy (STM), and Density Functional Theory (DFT), we examine the structural properties of (dehydrogenated) HHTP monolayers on Cu(111). Our analysis reveals distinct HHTP motifs and elucidates their interactions, providing deeper insights into the design of molecular architectures through controlled surface chemistry.

O 13.3 Mon 15:30 H8

**Optical and Electronic Properties of Epitaxial Lead Phthalocyanine Monolayers and Bilayers on Graphite and Graphene** — •Roman Forker, Marco Gruenewald, Matthias Spoddeck, and Torsten Fritz — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

The optical and electronic properties of the near-infrared absorber lead phthalocyanine (PbPc) on graphitic surfaces are measured by means of differential reflectance spectroscopy (DRS) and scanning tunneling spectroscopy (STS), respectively. This is corroborated by a thorough structural characterization using scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), demonstrating the similarity of the adlayer structures on graphite and graphene substrates. The dielectric function of PbPc monolayers (ML) extracted from our DRS measurements exhibits monomer character, and thus provides evidence that there is no significant electronic coupling between the molecular film and graphite or graphene. From 1 to 2 ML the dielectric function changes drastically, indicating the formation of physical dimers. Concomitantly, for PbPc bilayers the electronic properties are found to be caused by the formation of face-to-face stacked molecules, resulting in a splitting of the $\mathrm{d}I/\mathrm{d}V$-features associated with the PbPc HOMO and LUMO upon bilayer formation. Our results are compared to previous photoelectron spectroscopy data of this system, where a similar splitting of the HOMO-related features was reported.

O 13.4 Mon 15:45 H8

**Growth of N-heterocyclic carbenes on modified silicon surfaces** — •Marie-Louise Fraser[1], Milan Kubicki[1], Ankita Das[2], Mowpriya Das[2], Preeti Chahar[2], Martin Franz[1], Frank Glorius[2], and Mario Dähne[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Universität Münster, Organisch-Chemisches Institut, Münster, Germany

Today's semiconductor industry is mainly based on silicon, thus the growth of organic films on silicon surfaces is a highly promising research field. However, the high number of dangling bonds typically present on silicon surfaces renders them often less suitable for molecular growth. With surface modifications more suitable silicon substrates can be produced. One such modification is a rare earth silicide layer on the Si(111) surface enabling growth of highly ordered monolayers [1]. Another suitable substrate is Si(111) modified by boron, as demonstrated e.g. for N-heterocyclic carbenes (NHCs) [2]. NHCs have been demonstrated to be particularly promising ligands for surface modification and functionalization. Here, scanning tunneling microscopy is used to examine the growth of the NHC molecule BIMe on both boron and rare-earth modified Si(111) surfaces. On both substrates, films with coverages ranging from submonolayers to complete monolayers could be successfully grown, allowing the determination of the adsorption geometry and of the ordering behavior in the monolayer. [1] M. Kubicki et al., *J. Phys. Chem. C* **128**, 13347 (2024). [2] M. Franz et al., *Nat. Chem.* **13**, 828 (2021).

O 13.5 Mon 16:00 H8

**Imaging Dihydrogen Bond-Driven Assembly of Borazine on Au(111)** — •Matthias Zeilerbauer, Marco Thaler, Barbara Obwaller, Milan Ončák, and Laerte L. Patera — Universität Innsbruck, Austria

Dihydrogen bonding (DHB) is a peculiar type of attractive interaction occurring between a partially positively charged hydrogen atom and a partially negatively charged hydrogen atom. Borazine represents a prototypical molecule exhibiting dihydrogen bonding in both gas phase, as well as in its crystalline form. For borazine assemblies on solid surfaces, a direct observation and characterization of dihydrogen bonding has remained elusive, possibly due to an intricate interplay of substrate-molecule and intermolecular interactions. Here we present evidence of dihydrogen bonding occurring in borazine assemblies on a Au(111) surface. By means of low-temperature scanning tunneling microscopy, we unveiled distinct configurations, exhibiting single and double dihydrogen bonding. Density functional theory calculations elucidate the interplay between substrate adsorption and intermolecular interactions to stabilize the formation of borazine dimers on Au(111), being the building blocks for the formation of larger assemblies.

O 13.6 Mon 16:15 H8

**From Physical Trends to Structural Control: Insights into Phase Transition Times at Metal-Organic Interfaces** — •Anna Werkovits, Simon B. Hollweger, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Austria

At many metal-organic interfaces, molecules in the wetting layer undergo lying-standing transitions, significantly altering interface properties. Understanding the kinetics governing these transitions is essential for controlling structural evolution over time. This knowledge is particularly critical for tailoring interfaces based on either kinetically trapped or thermodynamically favoured structures.

To facilitate the design of interfaces, we develop a physically motivated surrogate model that estimates the phase transition times across a wide range of metal-organic interfaces. Using a systematic set of kinetic Monte Carlo simulations, incorporating variations in energetic landscapes and relative molecule sizes (representing hypothetical interface systems), we extract the physical relationships governing the timescales of phase transitions. These dependencies are analysed as functions of adsorption energies (lying and standing), kinetic barriers for reorientation and diffusion, molecule sizes, and environmental parameters such as temperature and pressure. This approach yields a formula that serves as a foundation for understanding trends, controlling structural evolution, and estimating timeframes for experiments and applications to ensure phase stability. Additionally, it enables the design of systems that remain stable over long periods, even in metastable states, advancing experimental and practical applications.

O 13.7 Mon 16:30 H8

**Controlled Ion Beam Deposition supplied by Electrospray (ES-CIBD) - enabling UHV deposition of large, reactive or fragile building blocks for functional nano-architectures** — •Andreas Walz$^{1,2}$, Annette Huettig$^{1,2}$, Michael Walz$^{1,2}$, Hartmut Schlichting$^{1,2}$, and Johannes V. Barth$^{2}$ — $^{1}$pureions GmbH, Gilching, Germany — $^{2}$Technical University of Munich, Germany

Cutting-edge research in the field surface- and nano- science using organic molecules requires control and unbiased understanding of structure and composition. Standard deposition techniques for the underlying building blocks restrict possible candidates: Thermal evaporation in vacuum (MBE, OMBE) is limited to volatile substances. Solution-based techniques such as drop casting, spin coating or inkjet printing are versatile but often lack purity and quality. Electrospray ionization (ESI) combined with mass selection and soft-landing of molecules unravels the vast potential of large, reactive or bio-relevant building blocks. The pool of possible molecules spans a wide spectrum from small organic molecules, over graphene nanoribbons (GNRs) up to several kilo- and megadalton proteins, DNA, but also inorganic clusters and larger nanoparticles may be possible. In-line with this, we present an UHV ion beam deposition device and its functionalities. Deposited layers are analyzed via STM. The main body of the device contains RF-driven ion guides with high transmission (>80% efficiency). A digital square-wave quadrupole mass filter (dQMF) provides virtually unlimited m/z-range. The footprint is benchtop in size, 0,5 x 1 m.

O 13.8 Mon 16:45 H8

**Reactions of benzoporphyrins with Cu(111)** — •Maximilian Muth, Majid Shaker, Julien Steffen, Alexander Wolfram, Simon Steinbach, Andreas Görling, Hans-Peter Steinrück, and Ole Lytken — Friedrich-Alexande-Universität Erlangen-Nürnberg, Germany

Porphyrins are molecules with many interesting properties that change upon adsorption on solid substrates. This can lead to something as simple as a change in conformation of the molecule or something more drastic as a reaction with - or catalyzed by - the substrate. We have focused on three molecules: free-base tetraphenyl trans-dibenzoporpyhrin, copper tetraphenyl transdibenzoporpyhrin and free-base tetraphenyl tetrabenzoporpyhrin adsorbed on Cu(111). Using temperature-programmed desorption, X-ray photoelectron spectroscopy, scanning tunneling microscopy and density-functional theory calculations, we have identified three reactions in the temperature range from 280 to 1000 K. In the first reaction step at 350 - 480 K the free-base benzoporphyrins react with copper atoms from the substrate, forming metalloporphyrins. At 480 - 650 K, the phenyl rings and pyrrole/benzo rings undergo a ring fusion reaction. Finally, at 650 - 950 K, the molecules polymerize and all remaining hydrogen atoms desorb from the surface as H2.

O 13.9 Mon 17:00 H8

**Supercharging Polymorphism of Organic/Inorganic Interfaces** — •Christoph Wachter and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Graz, 8010, Austria

The polymorphism of organic/inorganic interfaces heavily influences a multitude of their properties. Therefore, altering the polymorphism by changing the substrate or modifying the intermolecular interactions has been studied extensively. However, the extent to which charge transfer affects polymorphism has yet to be investigated systematically. Based on the hypothesis that there is a link between the band width of polymorphs and their relative energy, we expect that polymorphs with larger band width are preferred if charge is transferred uniformly across the organic monolayer.

Conversely, it is also possible for charge to localize in individual adsorbates instead of spreading out across the monolayer. Such localized charge transfer occurs when the electronic coupling of the organic molecules to each other and to the substrate is small. In that case the relation stated above is not well-defined anymore.

To investigate the impact of both localized and delocalized charge transfer on polymorphism, we employ density functional theory in conjunction with a machine-learning based structure search algorithm. To properly capture charge localization, we go beyond the standard semilocal functionals by utilizing hybrid functionals and report whether the expected relation still holds in the case of localized charge transfer.

O 13.10 Mon 17:15 H8

**Towards 2D metal-organic frameworks on weakly interacting substrates: FeDCA on coinage metals and Bi$_2$Se$_3$(111) surfaces** — •Anna Kurowská$^{1}$, Matthias Blatnik$^{1}$, Veronika Stará$^{1}$, Pavel Procházka$^{1}$, Čestmír Drašar$^{2}$, and Jan Čechal$^{1,3}$ — $^{1}$Central European Institute of Technology, Brno University of Technology — $^{2}$Faculty of Chemical technology, University of Pardubice — $^{3}$Institute of Physical Engineering, Brno University of Technology, Czech Republic

The formation of 2D metal-organic frameworks (MOFs) on a surface of topological insulator (TI) is a promising path to design quantum materials with exotic properties. MOFs featuring ferromagnetically coupled metal atoms are theoretically predicted to induce an exchange gap in the TI's surface band structure, potentially leading to a quantum anomalous Hall effect. However, the knowledge of self-assembly on TI substrates is still scarce. Here, we demonstrate the first experimental realization of 2D MOF, Fe-dicyanoanthracene (FeDCA), on the surface of a strong TI Bi2Se3. The structure and morphology were studied via scanning tunneling microscopy (STM) and low-energy electron microscopy (LEEM) and diffraction (LEED). We compare the growth of FeDCA on the Bi$_2$Se$_3$(111) surface with coinage metals and gr/Ir(111) surfaces, and discuss the conditions at which we obtain typical mixed Kagomé-honeycomb lattice and at which a new hexagonal lattice appears. The demonstration of 2D MOF/TI hybrid material presents a milestone on the way toward their application in fault-tolerant spin interconnects in future quantum devices.

# O 14: 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)

Time: Monday 15:00–18:00 Location: H11

O 14.1 Mon 15:00 H11

**Hexagonal structures of europium oxides on Pd(111) studied with LEED and STM** — •Muriel Wegner, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Germany

With an increasing interest in technological applications of oxide materials, also two-dimensional (2D) oxides came into focus. The large flexibility in the variation of the cationic species, including even a combination of different cations, promises a rich variety of properties [1,2]. So far, the center of attention has been on transition metal sesquioxides $M_2O_3$ of corundum structure.

Here, we expand this field towards lanthanides. We present a combined scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) study of the growth of submonolayer coverages of europium oxide on a Pd(111) surface. Upon annealing the as deposited Eu in oxygen containing environments at temperatures above 800 K, long-range ordered multilayer islands of $Eu_2O_3$ are obtained. From LEED a $\begin{pmatrix} 8/3 & 4/3 \\ -4/3 & 4/3 \end{pmatrix}$ superstructure on Pd(111) is derived, which corresponds to a hexagonal lattice with a lattice parameter of 6.35 Å. This structure exhibits a large stability range. Only upon annealing to 1175 K in UHV an additional (2×2) superstructure evolves, which is seen as a hexagonal array of pores at a distance of 12.70 Å in STM. By addition of small amounts of Ti atoms, the transformation into planar two-dimensional films is achieved. These mixed-metal oxides form a honeycomb lattice with a lattice parameter of 7.2 Å. In contrast to pristine $Eu_2O_3$, the Ti containing honeycomb can easily be resolved in STM.

[1] M. Van den Bossche, J. Goniakowski, and C. Noguera, Nanoscale **13**, 19500 (2021)
[2] P. I. Wemhoff, N. Nilius, C. Noguera, and J. Goniakowski, J. Phys. Chem. C **126** (10), 5070 (2022)

O 14.2 Mon 15:15 H11

**Growth of an Fe buckled honeycomb lattice on Be(0001)** — Hermann Osterhage[1], Abid H. Khan[2], Karoline Oetker[1], Radek Dao[1], Samaneh Setayandeh[2], Patrick Burr[2], Roland Wiesendanger[1], and •Stefan Krause[1] — [1]University of Hamburg, Germany — [2]University of New South Wales, Sydney, Australia

The Be(0001) surface is considered to be an ideal model system to host a 2D electron gas with pronounced electron-electron and electron-phonon interactions that are decoupled from the bulk [1,2]. In a combined scanning tunneling microscopy (STM) and density functional theory (DFT) study the growth of Fe on a clean Be(0001) surface is investigated on the atomic scale [3]. At low Fe coverage, the nucleation of terraced nanoislands with a disordered surface is observed experimentally with STM. Increasing the Fe coverage results in the growth of extended films exhibiting a well-ordered p(2×2) superstructure. DFT is applied to investigate the growth of Fe on a Be(0001) surface from individual atoms to extended films.

The Fe buckled honeycomb lattice formation on Be(0001), as derived from our study, provides evidence for the realization of a very peculiar non-trivial electronic and magnetic model system. The results will be presented and discussed in terms of their implications for the emergence of novel electronic and magnetic phases resulting from the interactions between the 2D electron gas and the magnetic atoms.

[1] P. T. Sprunger *et al.*, Science **275**, 1764 (1997).
[2] H. Osterhage *et al.*, Phys. Rev. B **103**, 155428 (2021).
[3] H. Osterhage *et al.*, Surf. Sci **752**, 122609 (2025).

O 14.3 Mon 15:30 H11

**Electronic structure and edge states in the 2D Kagome lattice $Ta_2S_3$ / Au(111)** — •Thais Chagas[1], Alessia Bardazzi[1], Samuel M. Vasconcelos[2], Alan C. R. Souza[3], Catherine Grover[1], Alice Bremerich[1], Kai Mehlich[1], Daniel Weber[1], Mario S. C. Mazzoni[3], Michael Rohlfing[2], and Carsten Busse[1] — [1]Department Physik, Universität Siegen, Germany — [2]Institute of Solid State Theory, Universität Münster, Germany — [3]Departamento de Física, Universidade Federal de Minas Gerais, Brazil

Kagome structures are a key model system in quantum physics, representing one of the most geometrically frustrated 2D magnetic lattices. In these systems, magnetic moments condense into a spin liquid phase at low temperatures, leading to intriguing physical phenomena. The characteristic Kagome bands in this lattice consist of a Dirac cone that gives rise to massless Dirac fermions with high mobility and a flat band that, in contrast, leads to fermions with infinite effective mass.

In this work, we investigate the 2D $Ta_2S_3$ Kagome phase on Au(111) using scanning tunneling microscopy (STM). STM images reveal bright island edges as a consequence of an enhanced density of states, indicating the presence of edge states. Additionally, we observe a significant dependence of atomic contrast on tunneling conditions, suggesting a complex electronic band structure near the Fermi level. Furthermore, we analyze the impact of growth parameters on defect formation. Finally, density functional theory (DFT) was employed to study the electronic structure of this material on Au(111), providing deeper insight into its electronic properties and interactions.

O 14.4 Mon 15:45 H11

**Spectroscopic and microscopic study of (car)borane based 2D materials** — •Martha Frey[1], Julian Picker[1], Jakub Visnak[2], Christof Neumann[1], Tomas Base[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, c.p. 1001, Czech Republic

Boranes are electron-delocalized molecular clusters containing boron and hydrogen. Their electron-deficient bonding and structural diversity as well as their high thermal stability make them attractive for applications ranging from optoelectronics to energy storage. Here we present the fabrication of a novel boron-based, carbon free two-dimensional (2D) material via electron-induced crosslinking of borane-based self-assembled monolayers (SAMs) on silver substrates. The SAMs, crosslinking process and resulting nanomembranes were analyzed using complementary surface-sensitive techniques including X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS), low-energy electron diffraction (LEED) and scanning tunneling and electron microscopies (STM, SEM). Furthermore, the results were compared with carborane-based 2D nanomaterials studied previously in our labs. The results demonstrate that properties of the 2D (car)borane nanosheets can be adjusted and tailored by the respective SAM constituents and that these structurally diverse cluster molecules open up new avenues for engineering novel functional 2D materials.

O 14.5 Mon 16:00 H11

**Growth and Structure of Titanium Ditelluride Films on Au(111)** — •Andreas Raabgrund, Alexander Wegerich, Lutz Hammer, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Aiming at the MBE growth of transition metal ditelluride ($MTe_2$) films particularly in the single-layer limit, the formation of and interaction with the interface is of fundamental interest. The growth of a $MTe_2$ film can be achieved either by the tellurization of the desired metal substrate [1] or by the reactive deposition of Te and the corresponding transition metal M on a suitable substrate [2].

In this contribution we follow the latter approach and investigate both single- and multilayer $TiTe_2$ films on Au(111) by LEED-IV, DFT, and STM. At first glance, LEED suggests a (4 × 4) superstructure with three $TiTe_2$ on four Au(111) unit cells. STM topography, however, reveals a mismatch of about 1% of the growing film w.r.t. the Au(111) substrate which indicates a relaxed $TiTe_2$ layer. LEED-IV results favor a film in close contact with Au substrate (Te-Au layer distance: $\approx 2.7$ Å). By DFT total energy calculations we find that neither Te nor Ti substitution is favored in the topmost Au layer. Continuing the reactive deposition of Ti and Te a multilayer $TiTe_2$ film grows epitaxially as found by LEED-IV with a Pendry R factor of 0.12. Further, we discuss the transferability of this growth recipe to other $MTe_2$ films on Au(111).

[1] T. Kißlinger et al., Phys. Rev. B **108**, 205412 (2023)
[2] K. Lasek et al., ACS Nano **14**, 8473 (2020)

O 14.6 Mon 16:15 H11

**Growth and Edge Reconstruction of 2D $MnI_2$ on Ag(111)** —

•Daniel Rothhardt[1,2,3], Christopher Penschke[4], Hans Josef Hug[1,2], Regina Hoffmann-Vogel[3], and Amina Kimouche[3] — [1]Empa, 8600 Dübendorf, Switzerland — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland — [3]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [4]Institute of Chemistry, University of Potsdam, 14476 Potsdam, Germany

The reduced dimensionality of thin transition metal dihalide films on single-crystal surfaces enables a wide array of magnetic and electronic phenomena. However, producing stoichiometric monolayer islands demands thorough control over growth parameters. In this work, we utilize scanning probe microscopy (SPM) to explore the growth of MnI$_2$ on Ag(111) through single-crucible evaporation. The Ag(111) surface's catalytic activity promotes dehalogenation of MnI$_2$, resulting in a reconstructed iodine adlayer that serves as a template for the formation of truncated hexagonal MnI$_2$ islands. These islands display alter-nating edge lengths and distinctive Kelvin potentials, as revealed by Kelvin Probe Force Microscopy (KPFM). Density Functional Theory (DFT) calculations corroborate the experimental observations, including island heights, lattice parameters, and edge formation energies for both pristine and reconstructed edges. The asymmetry in edge lengths arises from differences in formation energies, determined by the orientation (up or down) of iodine atoms at the edges, as confirmed by DFT.

O 14.7 Mon 16:30 H11

**Low defect density in MoS$_2$ monolayers grown on Au(111) by metal-organic chemical vapor deposition** — •Julian Picker, Ziyang Gan, Christof Neumann, Antony George, and Andrey Turchanin — Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena, Germany

Monolayers of transition metal dichalcogenides (TMDs) possess high potential for applications in novel electronic and optoelectronic devices and therefore the development of methods for their scalable growth is of high importance. Among different suggested approaches, metal-organic chemical vapor deposition (MOCVD) is the most promising one for technological applications because of its lower growth temperature compared to most other methods, e.g., conventional chemical vapor or atomic layer deposition (CVD, ALD). Here we demonstrate the epitaxial growth of MoS$_2$ monolayers on Au(111) by MOCVD at 450 °C. We confirm the high quality of the grown TMD monolayers down to the atomic scale using several complementary methods. These include Raman spectroscopy, non-contact atomic force microscopy (nc-AFM), X-ray photoelectron spectroscopy and scanning tunneling microscopy (STM). The topographic corrugation of the MoS$_2$ monolayer on Au(111), revealed in a moiré structure, was measured as 20 pm by nc-AFM. The estimated defect density calculated from STM images of the as-grown MoS$_2$ monolayers is in the order of $10^{12}$ vacancies/cm$^2$. The defects are mainly caused by single sulfur vacancies.

J. Picker *et al.*, Micron **186**, 103708 (2024).

O 14.8 Mon 16:45 H11

**Characterization of a large-scale single-domain MoS$_2$ monolayer** — •Fabian Schöttke[1], Luka Pirker[2], Martin Vondráček[3], Michaela Hanušová[2], Václav Valeš[3], Jan Honolka[3], Otakar Frank[2], Matěj Velický[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Münster, Germany — [2]J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Prague, Czech Republic — [3]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

To fully utilize the outstanding optical and electronic properties of single-layer transition metal dichalcogenide (TMDC) in devices, a perfect single-domain film is needed. From the wealth of available preparation methods, exfoliation seems to provide the highest film quality. This method, however, commonly results in small flakes within the micrometer regime only. Exfoliation onto, or assisted by, a Au(111) surface is able to result in large-scale single-domain samples of several millimeters in diameter. We experimentally confirm the high quality of a MoS$_2$ monolayer on Au(111) by characterizing several sample properties: optical appearance, long-range structural order, work function changes, and the occupied & unoccupied electronic structure. Optical inspection and diffraction patterns easily identify millimeter-sized single domains. The electronic structure of MoS$_2$ is clearly distinguished from Au(111) states, especially measured by inverse photoemission in the $L$ gap of Au(111). In summary, our experimental data of a MoS$_2$ monolayer exfoliated onto Au(111) demonstrate the capability of this procedure to produce large-scale single-domain TMDC samples.

O 14.9 Mon 17:00 H11

**Kinetics of borophene growth on Ir(111) via boron segregation from the bulk** — •Marin Petrović[1], Sherif Kamal[1], Borna Radatović[1], Marko Kralj[1], Matteo Jugovac[2], Iulia Cojocariu[2], Andrea Locatelli[2], and Tevfik Onur Menteş[2] — [1]Centre for Advanced Laser Techniques, Institute of Physics, 10000 Zagreb, Croatia — [2]Elettra - Sincrotrone Trieste S.C.p.A, 34149 Trieste, Italy

Segregation of boron atoms to the Ir(111) surface and their self-assembly into a borophene monolayer were tracked by low-energy electron microscopy (LEEM). Real-time monitoring of sample temperature, boron adatom concentration and borophene coverage reveals the kinetics of boron segregation from the iridium bulk and different modalities of borophene epitaxial growth. It is found that the temperature-triggered boron segregation to the surface is accompanied by instantaneous nucleation of borophene islands and condensation of boron adatoms, followed by rapid propagation of island perimeter along the iridium terraces. Subsequent growth of borophene proceeds by displacement of iridium surface steps, which is energetically expensive and thus relatively slow process that heavily depends on the step morphology. By identifying and analyzing quasi-equilibrium conditions on the sample surface during borophene growth, formation enthalpy of a boron monomer from borophene was estimated, which agrees well with the available theoretical calculations of the boron-iridium system.

O 14.10 Mon 17:15 H11

**Growth and etching of hBN on Cu(111): Impact on substrate step dynamics and morphology** — •Patrick Seleš[1,2], Marin Petrović[1], Smruti Ranjan Mohanty[3], and Frank Meyer zu Heringdorf[3] — [1]Center for Advanced Laser Techniques, Institute of Physics, Bijenička 46, Zagreb, Croatia — [2]Faculty of physics, University of Rijeka, Radmile Matejčić 2, Rijeka, Croatia — [3]Faculty for Physics, University of Duisburg-Essen, Lotharstrasse 1-21, Duisburg, Germany

The interaction of precursors and oxygen molecules with metal surfaces plays an important role in the growth dynamics of two-dimensional material such as graphene and hexagonal boron nitride (hBN). By using low-energy electron microscopy (LEEM), in this study we investigate the influence of hBN growth on Cu(111) step dynamics at various stages ranging from borazine precursor dosing to oxygen etching. Real-time monitoring of Cu step displacement underneath and next to hBN islands revealed step pinning and a significant decrease in step velocities compared to the pristine Cu surface, highlighting the stabilizing effect of hBN. After the removal of hBN islands by oxygen etching, Cu steps accelerated back to the pre-growth velocities and rearranged into a new surface morphology. Our findings elucidate the interplay between surface dynamics and step motion during hBN growth on Cu(111). By analyzing step displacement and morphological evolution, we contribute to a deeper understanding of metal-catalyzed chemical vapor deposition growth of hBN.

O 14.11 Mon 17:30 H11

**In-situ growth and characterization of 2D TaSe$_2$ on Au(111)** — •Cathy Sulaiman[1], Lars Buss[1], Raquel Sánchez-Barquilla[1], Jens Falta[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Institute for Solid State Physics, University of Bremen, Bremen, Germany

Group V dichalcogenides such as Ta$X_2$ (X = S, Se, T) have extensively been investigated in recent decades due to their diverse electron correlation effects, including the occurrence of charge density waves and Mott-Hubbard transitions. In 2D, two polytypes, 1T and 1H, exist, which exhibit distinct properties, making selective growth of each polytype crucial. Using low-energy electron microscopy (LEEM), we have successfully observed the growth of two TaSe$_2$ phases on Au(111) *in situ* after the co-deposition of Ta and Se. At elevated temperature, micron-sized, triangle-shaped islands with bright contrast nucleate first and grow at a higher rate. However, this phase turns out to be metastable as it suddenly transitions into a more stable phase (with dark contrast) and continues to grow at a reduced rate. Low-energy electron diffraction shows the presence of TaSe$_2$; bandstructure-sensitive I(V)-LEEM analysis reveals substantial differences in electron reflectivity between both phases. A comparison with TaS$_2$ suggests that the metastable and stable phases are 1T- and 1H-TaSe$_2$, respectively.

O 14.12 Mon 17:45 H11

**CVD growth of monolayer transition metal dichalcogenides heterostructures using liquid precursors** — •Md Tarik Hossain[1], Axel Printschler[1], Julian Picker[1], Christof Neumann[1], Moritz Quincke[2], Johannes Biskupek[2], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena 07743, Germany — [2]Central Facility of Electron Microscopy, Electron Microscopy Group of Material Science, University of Ulm, Ulm 89081, Germany

Heterostructures (HSs) formed of transition metal dichalcogenide (TMD) monolayers have attracted substantial research interest due to their unique physical properties. However, engineering the HS configurations (lateral and vertical) including the domain size for each TMD remains challenging. Here we present a facile route for the synthesis of different types of HSs of TMD monolayers using liquid precursors for transition metals. We characterized the TMD HSs by several complementary spectroscopy and microscopy techniques. Our results suggest that the HS configurations, lateral length and area of each TMD can be tuned by varying concentration ratios of the precursors. In addition, the overall heterostructure sizes can also be tuned from few to hundreds of micrometers. The developed method paves the way to obtaining high-quality lateral and vertical HS of $MoSe_2$-$WSe_2$ with controllable domain sizes.

## O 15: Focus Session Many-Body Phenomena in Nanomagnets: Kondo, Spinons, Spinarons and Beyond (joint session O/TT)

The electron spin, a fundamental quantum mechanical property, plays a crucial role in determining the electronic and magnetic properties as well as the dynamics of matter. Its role becomes even more important at surfaces, 2D materials and nanomagnets as the low-dimensionality increases electron correlation. A fundamental understanding of spin excitations is significant for both fundamental science and modern applications. For decades, the interpretation of experimental signatures of spin excitations were focused on the Kondo effect paradigm, with Co atoms on the (111) surface of noble metals as the prototypical example. However, recent first-principles predictions and spin-polarized scanning tunnelling spectroscopy in high magnetic fields have demonstrated the existence of many-body states, called spinarons. These states arise from the binding of electronic states to spin excitations in the presence of spin-orbit coupling. Such findings, along with other studies, challenge the Kondo interpretation. Furthermore, related nontrivial many-body states may emerge in thin-film geometries, as shown by photoemission spectroscopy and first-principles manybody investigations or in quantum spin liquids. These examples testify that many-body phenomena are not only critically important for the fundamental understanding of spin excitations, they also impact a wide range of material characteristics, including electronic, magnetic, thermodynamic, and transport properties. This focus session will provide a forum to discuss intriguing many-body states driven by spin excitations, and serve as a forum to discuss the current knowledge on their origins, unique properties, and implications.

Organized by
Matthias Bode (Würzburg University), Yujeong Bae (Swiss EMPA), and Stefan Blügel (FZ-Jülich).

Time: Monday 15:00–18:15 Location: H24

**Invited Talk** O 15.1 Mon 15:00 H24
**Kondo and Yu-Shiba-Rusinov resonances: transport and coupling** — •Laëtitia Farinacci[1,2,3], Gelavizh Ahmadi[3], Gaël Reecht[3], Benjamin W. Heinrich[3], Contanstin Czekelius[3], Felix von Oppen[3], and Katharina J. Franke[3] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena-Stuttgart-Ulm, Germany — [3]Fachbereich Physik, Freie Universität Berlin, Germany

The exchange coupling between a magnetic impurity and a superconducting substrate leads to the formation of magnetic bound states, known as Yu-Shiba-Rusinov (YSR) states, inside the superconducting gap, as well as a Kondo resonance outside the gap. Studying these two many-body phenomena in parallel provides valuable insights into their characteristic properties.

We observed striking correlations between the asymmetries of the YSR state and the Kondo effect induced by FeTPyP molecules on Pb(111) in a scanning tunneling microscope (STM) [1]. We show that both asymmetries originate from interfering tunneling paths via a spin-carrying orbital and the highest occupied molecular orbital.

Additionally, we studied the formation of YSR bands in a self-assembled kagome lattice of magnetic molecules on Pb(111) and track YSR hybridization from kagome precursors to larger islands [2]. This work will motivate further studies to resolve possible spin-liquid or Kondo-lattice-type behavior.

[1] PRL 125, 256805 (2020). [2] Nat. Comm. 15, 6474 (2024).

**Invited Talk** O 15.2 Mon 15:30 H24
**Electron delocalization in a 2D Mott insulator** — •Amadeo L. Vazquez de Parga[1,2,4,5], Cosme G. Ayani[1,2], Michele Pisarra[3], Iván M. Ibarburu[1], Clara Rebanal[1], Manuela Garnica[2,4], Fabián Calleja[2], and Fernando Martín[1,2] — [1]Universidad Autónoma de Madrid, Madrid, Spain — [2]IMDEA Nanociencia, Madrid, Spain — [3]Universitá della Calabria, Rende, Italy — [4]Instituto Nicolás Cabrera, Madrid, Spain — [5]Condensed Matter Physics Center (IFIMAC), Madrid, Spain

We follow by means of low temperature Scanning Tunneling Microscopy and Spectroscopy, the buildup of a 2D Kondo lattice in a system composed by a 2D Mott insulator, a single 1T-TaS2 layer, stacked on the surface of a metallic crystal, 2H-TaS2. When the sample temperature is lower than 27K, the magnetic moments present in the Mott insulator experience the Kondo screening by the conduction electrons of the metal, leading to the appearance of a Kondo resonance at the Fermi level. Below 11 K, a gap opens within the Kondo resonance, which is the signature of the formation of a coherent quantum state that extends all over the sample, i.e., a Kondo lattice [1]. Quasi particles interference maps reveal the emergence of a Fermi contour in the 2D Mott insulator when the temperature drops below 11K, indicating the delocalization of the highly correlated Mott electrons [2]. The observed modifications in the LDOS are well explained by state-of-the-art Density Functional Theory calculations.

[1] Small 20, 2303275 (2024) [2] Nat. Commun. 15, 10272 (2024)

**Invited Talk** O 15.3 Mon 16:00 H24
**Kondo or no Kondo, that is the question** — •Alexander Weismann, Neda Noei, Niklas Ide, and Richard Berndt — Institut für experimentelle und angewandte Physik, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

The spin properties of individual atoms and molecules can produce distinctive spectral features in tunneling spectra near zero bias. Among these features, Kondo resonances and inelastic spin-flip excitations are often challenging to distinguish, despite their markedly different spectral line shapes. A Kondo resonance indicates a non-magnetic ground state, where the atomic spin is screened by conduction band electrons.

In contrast, spin-flip excitations observed in zero-field tunneling spectra require magnetic anisotropy, which arises from spin-orbit coupling (SOC), to play a significant role. In this study, we demonstrate that the well-known Co/Cu(111) system, long believed to exhibit a Kondo resonance, instead adopts a magnetic ground state that is protected from Kondo screening by substantial magnetic anisotropy. The zero-bias anomaly in scanning tunneling spectra undergoes significant modification when Co atoms are attached to monoatomic Cu chains. Measurements conducted at 340 mK in a magnetic vector field reveal clear signatures of inelastic spin-flip excitations, with the anisotropy axis tilted away from the surface normal. The magnitude and orientation of this anisotropy are consistent with density functional theory (DFT) calculations. Moreover, quantum Monte Carlo many-body simulations confirm that the Kondo effect is suppressed when SOC is properly accounted for.

**Invited Talk** O 15.4 Mon 16:30 H24

**Evidence for spinarons in Co atoms on noble metal (111) surfaces** — •Artem Odobesko — Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg

The zero-bias anomaly in the tunnelling differential conductance of Co atoms on Au(111) [1], long attributed to the Kondo effect, has recently been reinterpreted [2] as evidence of the spinaron – a novel many-body excitation arising from the interplay between spin excitations and conduction electrons. In our study, we used spin-polarized scanning tunneling spectroscopy (STS) on Co atoms on Cu(111) and Au(111) under high magnetic fields, revealing field-induced energy shifts and spin-resolved spectral features that challenge the conventional Kondo interpretation. Instead, our findings provide the first experimental confirmation of the spinaron [3].

We also investigated the role of hybridization with the substrate in spinaron formation, focusing on the reconstructed Au(111) surface. The unique local electronic environments created by the herringbone reconstruction strongly influence the hybridization strength and spectral features of Co adatoms, revealing a clear link between adsorption site, hybridization, and spinaronic excitations. Our results shed light on the fundamental mechanisms driving spinaron formation.

[1] V. Madhavan, et al., Science 280, 567 (1998)
[2] J. Bouaziz, et al., Nat. Comm. 11, 6112 (2020)
[3] F. Friedrich, et al., Nat. Phys. (2023)

**Invited Talk** O 15.5 Mon 17:00 H24

**Spinarons: A new view on emerging spin-driven many-body phenomena in nanostructures** — •Samir Lounis — Peter Grünberg Institut, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany — Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle (Saale), Germany

Many-body phenomena are crucial in physics, particularly in condensed matter, influencing electronic, magnetic, thermodynamic, and transport properties. They leave distinct spectroscopic signatures, such as Kondo, excitonic, and polaronic features, arising from specific degrees of freedom. Since more than two decades Cobalt atoms on the (111) surfaces of noble metals have been a paradigm for the Kondo effect in scanning tunnelling spectroscopy experiments [1]. However, our recent first-principles predictions [2] followed by STS experiments in high magnetic fields [3,4] challenge this notion. Our findings reveal that the observed transport anomalies stem from spin excitations of Co atoms, forming a new many-body state – the spinaron – distinct from the Kondo resonance. I will delve into the spinaron origins, their unique properties, and implications explored through the recent atomic manipulation experiments. This work opens pathways to investigate and engineer these hybrid states in nanostructures, offering new insights into fundamental many-body states.

[1] V. Madhavan et al., Science 280, 567 (1998); [2] J. Bouaziz et al., Nat. Commun. 11, 6112 (2020); [3] F. Friedrich et al., Nat. Phys. 20, 28 (2024); [4] N. Noei et al., Nanoletters 23, 8988 (2023)

O 15.6 Mon 17:30 H24

**Emergence of spinaronic states in Fe adatoms** — Ilias Klepetsanis[1,2], Juba Bouaziz[4], •Philipp Rüssman[1,3], and Samir Lounis[1,2] — [1]Forschungszentrum Jülich & JARA, Germany — [2]University of Duisburg-Essen and CENIDE, Germany — [3]University of Würzburg, Germany — [4]Research Center for Advanced Science and Technology, University of Tokyo, Japan

In recent years, spinarons, predicted from first-principles calculations [1], have been observed in Co adatoms on the Cu(111) surface, using spin-polarized scanning tunnelling spectroscopy (STS) in high magnetic fields [2]. Spinarons leave a non-trivial spectroscopic signature, for long interpreted to originate from the Kondo effect [3]. Here, we employ relativistic time-dependent density functional and many-body perturbation theory, to investigate the case of Fe adatoms on the Cu(111) surface, which carry a large magnetic moment of $3.25\mu_B$ preferring an out-of-plane orientation as dictated by a magnetic anisotropy energy of 2meV. In contrast to the Co adatom, the spinarons in Fe do not overlap with trivial spin-excitations. We discuss the spinaronic response to an out-of-plane magnetic field, the orbital character and the impact of spin-orbit coupling. [1] J. Bouaziz et al., Nat. Commun. 11, 6112 (2020); [2] F. Friedrich et al., Nat. Phys. 20, 28 (2024); [3] V. Madhavan et al., Science 280, 567 (1998)

O 15.7 Mon 17:45 H24

**Revising the Superconductivity in Iron Based Superconductors from the Perspective of Electron Phonon Coupling** — •Lanlin Du[1,2] and Sheng Meng[1,2,3] — [1]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing, China — [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing, China — [3]Songshan Lake Materials Laboratory, Dongguan, Guangdong, China

There are currently two mainstream superconducting pairing mechanisms, namely electron phonon coupling and spin fluctuation, which are believed to play a dominant role in conventional superconductors like simple metal superconductors and unconventional superconductors like Copper oxides, respectively. Iron based superconductors are believed to connect these two aspects, that is, both mechanisms are important in it. In fact, some studies have shown that electron phonon coupling is also important in cuprates, and even provide evidence for s-wave pairing symmetry in them. Therefore, it is important to consider the role of electron phonon coupling in unconventional superconductors. Here, we revise the superconductivity in Iron based superconductors using Migdal-Eliashberg formalism and electron phonon coupling strength corrected by many body method from the two perspectives of doping and pressurization. Our results are in good agreement with the experiments. Based on this, we predict a new two-dimensional high-Tc Iron based superconductor.

O 15.8 Mon 18:00 H24

**Theoretical model for multiorbital Kondo screening in strongly correlated molecules with several unpaired electrons** — •Manish Kumar[1], Aitor Calvo-Fernandez[2], Diego Solar-Polo[1], Asier Eiguren[2], Maria Blanco-Rey[3], and Pavel Jelinek[1] — [1]Institute of Physics, Academy of Sciences of the Czech Republic , Cukrovarnicka 10, Prague 6, CZ 16200, Czech Republic — [2]Department of Physics, University of the Basque Country UPV-EHU, 48080 Leioa, Spain — [3]Department of Polymers and Advanced Materials: Physics, Chemistry and Technology, University of the Basque Country UPV-EHU, 20018 Donostia-San Sebastián, Spain

The mechanism of Kondo screening in strongly correlated molecules with several unpaired electrons on a metal surface is still under debate. Here, we provide a theoretical framework that rationalizes the emergence of Kondo screening involving several extended molecular orbitals with unpaired electrons. We introduce a perturbative model, which provides simple rules to identify the presence of antiferromagnetic spin-flip channels involving charged molecular multiplets responsible for Kondo screening. The Kondo regime is confirmed by numerical renormalization group calculations. In addition, we introduce the concept of Kondo orbitals as molecular orbitals associated with the Kondo screening process, which provide a direct interpretation of experimental dI/dV maps of Kondo resonances. We demonstrate that this theoretical framework can be applied to different strongly correlated open-shell molecules on metal surfaces, obtaining good agreement with previously published experimental data.

# O 16: Scanning Probe Techniques: Method Development

Time: Monday 15:00–18:00 Location: H25

O 16.1 Mon 15:00 H25

**Fast and quantitative nanomechanical mapping using photothermal off-resonance tapping atomic force microscopy (AFM)** — •Gunstheimer Hans[1,2], Fläschner Gotthold[1], Adams Jonathan[1], Hölscher Hendrik[2], and Hoogenboom Bart[1] — [1]Nanosurf AG, Gräubernstrasse 12-14, 4410 Liestal, Switzerland — [2]Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology, Karlsruhe, Germany

Multifunctional imaging, makes AFM a powerful tool for nanoscale surface analysis. However, most scanner-based methods for measuring mechanical properties are slow, limiting their use in fast mapping of mechanical characteristics. The main source of limitation is the piezo scanner, used to modulate tip-sample distance. This can be overcome by direct cantilever actuation, such as photothermal excitation. By moving the cantilever's comparably smaller mass, higher actuation bandwidths are accessible, enabling new approaches for AFM-based nanomechanical characterization. Here, we share insights on applying photothermal off-resonance tapping to fast nanomechanical property mapping. Based on simulations of cantilever bending due to laser-induced heating, we predict the cantilever response and propose a procedure to convert thermomechanical cantilever behavior into a calibrated nanomechanical measurement. We present the experimental method validation by measurements of polymer samples and reference structures. This novel photothermal off-resonance tapping mode enables quantitative nanomechanical mapping at frequencies of several tens of kHz, unlocking new insights into dynamic sample behavior.

O 16.2 Mon 15:15 H25

**Multifrequency Excitation and High Dynamic Range Tunneling Spectroscopy** — Philipp E.J. Maier, Ajla Karić, Carolina A. Marques, Berk Zengin, and •Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

The massive number of spectra required for high-resolution quasiparticle interference of low-dimensional quantum materials motivates the development of faster point spectroscopies. While the advent of parallel spectroscopy and compressive sensing enhancements has provided welcome speed boosts, these come at a cost. The application of a sinusoidal voltage on the nonlinearities in the current-voltage characteristics of a tunneling junction generates a frequency comb of higher order current-harmonics. While their parallel measurement enables faster tunneling spectroscopy, it unfortunately averages longest where the currents are largest, leading to poor signal-to-noise ratios for smaller signals associated with features close to the Fermi level. Here, we introduce a multifrequency excitation mode that increases the averaging time for small currents, enabling fast and high-resolution spectroscopy. Additionally, the AC excitation of our method can be used to dramatically increase the dynamical current range by exactly and deliberately suppressing the large amplitude, low order harmonics that would otherwise saturate the preamplifier stage.

O 16.3 Mon 15:30 H25

**Dynamics on the atomic-scale: Use and limitations of stochastic resonance spectroscopy** — •Nicolaj Betz[1,2], Vivek K. Rajathilakam[1], Laëtitia Farinacci[1,3], Susan N. Coppersmith[4], 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]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena-Stuttgart-Ulm, Germany — [4]School of Physics, University of New South Wales, Sydney, Australia.

Stochastic dynamics offer valuable insight into the internal structure of a system and its interactions with the environment. However, in atomic-scale systems investigated using scanning tunneling microscopy, comprehensive and accurate characterization is often a significant challenge. In this talk, we discuss a new type of measurement technique, stochastic resonance spectroscopy (SRS), that provides comparatively large signals over a wide range of timescales down to the picosecond range. It uses the effect of stochastic resonance, where the system's state synchronizes with an external harmonic drive. This encodes information about the dynamics in a time-independent signal. Such drive-induced imprinting of time-independent signals can alter the system's dynamics, but this limitation can be mitigated in SRS by its ability to identify and even tune these drive-induced dynamics. This enables targeted investigation of driven quantum systems on the atomic scale.

O 16.4 Mon 15:45 H25

**From experiments to insights: processing tool for SPM images with periodic pattern** — •Farzin Irandoost[1], Fillippo Federici Canova[2], Tobias Dickbreder[3], Franziska Sabath[3], Angelika Kühnle[3], and Adam S. Foster[1,4] — [1]Department of Applied Physics, Aalto University, Helsinki, Finland — [2]Nanolayers Research Computing Ltd., London, England — [3]Physical Chemistry I, Bielefeld University, Germany — [4]Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Japan

Big datasets of Scanning Probe Microscopy (SPM) images are potentially valuable, but robust algorithms are required for preprocessing them due to the high levels of defects and noise introduced during experiments. These issues often render many images unusable, especially for in-liquid SPM studies.

As part of a study on hydration patterns using a dataset of in-liquid calcite, we developed a versatile workflow to clean the data and extract features for further analysis. This workflow automatically corrects non-linear defects, ensuring the outputs closely resemble ideal periodic patterns. Consequently, many previously discarded raw images can be recovered to prepare a large, clean dataset ready for analysis. Afterward, the features of interest could be extracted using pattern decomposition facilitated by Fourier transforms.

This approach provides access to invaluable information about the lattice and hydration patterns for our study. Additionally, it offers a versatile tool for broader analyses of images with periodic structures.

O 16.5 Mon 16:00 H25

**True Alternating Current Scanning Tunneling Microscope (ACSTM): tunneling on insulators** — •Marcel Rost[1] and Milan Allan[1,2] — [1]Leiden Institute of Physics (LION), Leiden, NL — [2]University of Munich (LMU), Munich, Germany

Scanning Tunneling Microscopy has revolutionized our atomic scale understanding of surfaces and accelerated progress in nanotechnology. This technique, however, is restricted to metal or semiconducting samples, as it requires a tiny current to stabilize the tip-sample distance with atomic scale precision.

We developed a new imaging and feedback method that relies on true alternating current (AC) without any direct current (DC) component. This technique does not only enable the imaging on non-conducting surfaces with atomic resolution, like (thin) glass and oxides, it provides also access to high-frequency electronic sample information. We demonstrate that it is possible to measure on 22nm thick silicon oxide with 10 MHz tunneling current.

O 16.6 Mon 16:15 H25

**STM-induced luminescence with a parabolic mirror - millions of counts** — •Yannis Hilgers, Andreas Reutter, Mike Stummvoll, Markus Etzkorn, and Uta Schlickum — Institute of Applied Physics - LENA, TU Braunschweig, Germany

In recent years, scanning tunneling microscopy-induced luminescence (STML) has become a powerful technique allowing to record topography with atomic resolution and simultaneous spatially resolved photon count maps. We have built a Photon STM with a large parabolic mirror which was specifically designed for high photon collection efficiency. With this system we detected so far unreached photon counts of about 6 million photons per second at 1 nA tunnelling current that result from the decay of plasmon-polariton excitations between a Ag(111) surface and a Ag tip. Considering losses due to geometry, shadowing, optical components and detectors, we estimate a yield of approximately $5 \cdot 10^{-3}$ photons per tunnelling electron. This is scratching on the theoretical predictions by Johansson et al. [1], Persson and Baratoff [2] and others who all reported conversion factors in the range of $10^{-4}$ to $10^{-3}$ at most. In this talk we discuss these results, the instrumental calibrations and assumptions necessary for this estimation and speculate about possible explanations of the high observed excitation efficiency.

1 P. Johansson, R. Monreal, P. Apell - Phys. Rev. B 42, 9210 (1990)
2 B.N.J. Persson, A. Baratoff - Phys. Rev. Lett. 68, 3224 (1992)

O 16.7 Mon 16:30 H25

**Momentum-polarized microscopy with van der Waals scanning probe tip.** — •Abhisek Kole[1,2,4], Frank Stefan Tautz[1,2,4], Markus Ternes[1,2,3], Jose Martinez Castro[1,2,3], and Felix Lüpke[1,2,5] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, Germany — [3]Institut fur Experimentalphysik II B, RWTH Aachen, Aachen, Germany — [4]Institut fur Experimentalphysik IV A, RWTH Aachen, Aachen, Germany — [5]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany

Van der Waals materials are celebrated for their remarkable 2D physics, which includes correlated phenomena and topological effects. In this work, we present momentum-polarized microscopy using a van der Waals scanning probe tip. We developed and implemented a novel fabrication method to fabricate van der Waals scanning tunneling tips from exfoliated graphite flakes. The fabricated tips were characterized by atomically resolved scanning tunneling microscopy (STM) on an Ag(111) surface, where differential conductance measurements provided direct evidence of tunneling through the zigzag edge states of graphene. In addition, Friedel oscillations on the Ag(111) surface revealed clear signs of momentum-dependent tunneling, manifesting as anisotropic tunneling conductance. To further validate and investigate the momentum selective properties of the zigzag graphene tips, we have resolved the momentum dependent superconducting gap on FeSe lattices.

O 16.8 Mon 16:45 H25

**Image-to-molecule translation for high-resolution SPM images** — •Lauri Kurki[1], Jie Huang[1], Niko Oinonen[1,2], and Adam S. Foster[1,3] — [1]Aalto University, Finland — [2]Nanolayers Research Computing Ltd., UK — [3]WPI-NanoLSI, Kanazawa University, Japan

Scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) functionalized with a CO molecule on the probe apex capture sub-molecular level detail of the imaged sample [1]. However, the produced images are often difficult to interpret due to complex tip-sample interactions. To accelerate image analysis, we propose machine learning tools to extract sample properties directly from SPM images.

In recent years, there has been rapid development in image analysis methods in SPM in general and in particular for extracting atomic positions from AFM and STM images [2,3,4]. We build upon these models and achieve improved chemical and physical sensitivity compared to previous results [2]. Additionally, we explore equivariant neural networks [5] and compare their data efficiency and accuracy to traditional deep learning models.

[1] Cai et al., J. Am. Chem. Soc. 2022, 144, 44, 20227-20231 [2] Kurki et al., ACS Nano 2024, 18, 17, 11130*11138 [3] Alldritt et al., Sci. Adv. 2020; 6 : eaay6913 [4] Carracedo-Cosme et al., Nanomaterials 2021, 11, 1658. [5] Cesa et al., arXiv:1911.08251

O 16.9 Mon 17:00 H25

**Scanning Quantum Microscopy for 2D Superconductors** — •Ruoming Peng[1], Malik Lenger[1], Sreehari Jayaram[1], and Joerg Wrachtrup[1,2] — [1]3. Physikalisches Institut, University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Visualization of nanoscale dynamics in 2D superconductors provides critical insights into pairing mechanisms and topological electronic responses. Using state-of-the-art scanning quantum microscopy based on nitrogen-vacancy (NV) centers in diamonds, we investigate the local magnetic behavior of the 2D superconductor 2H-NbSe2 with high sensitivity and spatial resolution. This approach enables the first spatial-temporal measurements of vortex dynamics in thin exfoliated 2H-NbSe2, revealing a strong correlation between vortex arrangements and geometric confinement. We observe the melting transition of vortex solids near the critical temperature, alongside cooling-rate-dependent vortex rearrangements across thermal cycles. Additionally, through local magnetic noise probing via spin coherence time (T2) measurements, we uncover unexpected supercurrent fluctuations in reduced dimensionality. These findings highlight the potential of scanning quantum microscopy in advancing our understanding of vortex physics and emergent phenomena in 2D superconducting systems.

O 16.10 Mon 17:15 H25

**A high-throughput ESR-STM setup at mK temperatures** — •Máté Stark, Jonas Arnold, Luise Renz, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Characterizing and controlling single spins using Electron Spin Resonance Scanning Tunneling Microscopy (ESR-STM) [1] benefits from ultra-low temperatures, minimal noise, and efficient RF transmission to the junction. This work details upgrades to an ESR-STM system operating at mK temperatures within a compact dilution refrigerator under UHV conditions. We achieved an electronic temperature below 200 mK while maintaining effective RF transmission up to 40 GHz. In addition, we developed a compact UHV chamber with an automated sputter-annealing stage, allowing for efficient sample preparation and quick exchange of samples with various atoms and molecules atop. In combination with the fast cooldown of the dilution refrigerator, these upgrades greatly streamline the experimental workflows allowing for rapid and high quality ESR-STM measurements. [1] Baumann, S. et al., 350(6259), 2015.

O 16.11 Mon 17:30 H25

**Molecular Identification via Molecular Fingerprint extraction from Atomic Force Microscopy images** — •Manuel González Lastre[1], Pablo Pou[1,2], Miguel Wiche[3,4], Daniel Ebeling[3,4], Andre Schirmeisen[3,4], and Rubén Pérez[1,2] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Spain — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Institute of Applied Physics, Justus Liebig University Giessen, Giessen, Germany — [4]Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany

Previous works have already shown that deep learning (DL) models can retrieve the chemical and structural information encoded in a 3D stack of constant-height HR–AFM images, leading to molecular identification.

In this work, we overcome their limitations by using a well-established description of the molecular structure in terms of topological fingerprints, the Extended Connectivity Fingerprints, which provide local structural information of the molecule. In this work, we train a DL model to extract this optimized structural descriptor from the 3D HR–AFM stacks and use it, through virtual screening, to identify molecules from their predicted ECFP4 with a retrieval accuracy on theoretical images of 95.4%. This approach, unlike previous DL models, assigns a confidence score, the Tanimoto similarity, to each of the candidate molecules, thus providing information on the reliability of the identification.

O 16.12 Mon 17:45 H25

**The Josephson effect in the dynamical Coulomb blockade regime with high energy resolution** — •Xianzhe Zeng[1], Janis Siebrecht[1], Haonan Huang[1], Sujoy Karan[1], Klaus Kern[1,2], and Christian R. Ast[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The Josephson effect can be used as a good quantitative indicator of the energy resolution of scanning tunneling microscopy (STM). Recently we have upgraded our mK-STM with low-temperature filtering on our scan head. We measured the Josephson current and found an improvement of the energy resolution by almost an order of magnitude. The high resolution allows us to measure several spectroscopic features in detail, including the superconducting coherence peaks with extreme sharpness and the environmental resonances in the Josephson current at low frequency due to the dynamical Coulomb blockade.

# O 17: Poster Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation

Time: Monday 18:00–20:00 Location: P2

O 17.1 Mon 18:00 P2

**Synthesis and characterization of a non-planar cyclophenylene on Au(111)** — Sergio Salaverria[1], Martin Irizar[2,3,4], Jesus Janeiro[5], Paula Angulo-Portugal[6], Tao Wang[2], Jan Patrick Calupitan[6], •Jonathan Rodriguez-Fernandez[1,7], Aran Garcia-Lekue[2,8], Martina Corso[6], Emilio Artacho[2,3,8,9], Diego Peña[5], Dolores Perez[5], and Dimas G. de Oteyza[1,2] — [1]CINN, CSIC-UNIOVI-PA, El Entrego, Spain — [2]DIPC,San Sebastián, Spain — [3]CIC nanoGUNE, San Sebastián, Spain — [4]PMAS, UPV/EHU, San Sebastián, Spain — [5]CiQUS, Universidade de Santiago de Compostela, Spain — [6]CFM-MPC, CSIC-UPV/EHU, San Sebastián, Spain — [7]Physics Department, University of Oviedo, Spain — [8]Ikerbasque, Basque Foundation for Science, Bilbao, Spain — [9]TCM, University of Cambridge, Cambridge (UK)

Cyclophenylenes, i.e., macrocycles composed of linked benzene rings, have attracted intensive interest because of their appealing structures and potential applications.

In this work, we report the on-surface synthesis of a non-planar Au-coordinated cyclophenylene, containing four meta- and two para-connections, on a Au(111) surface, by undergoing hierarchical, metal-assisted double Ullmann coupling of a 1,10-dibrominated angular phenylene, and subsequent selective C-C bond cleavage of the four-membered rings in the resulting phenylene dimer. The chemical structure was characterized by bond-resolving (BR) STM and further supported by STS and DFT. This study offers the first approach for the synthesis of non-planar cyclophenylenes on surfaces.

O 17.2 Mon 18:00 P2

**Experimental benchmark for configuration monitoring during scanning-probe-microscope manipulation** — •Mong-Wen Gu[1], Jonas Lederer[2], Joshua Scheidt[1,2], Hadi H. Arefi[1], Kristof T. Schütt[2], Michael Gastegger[2], F. Stefan Tautz[1], Klaus-Robert Müller[2], and Christian Wagner[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany — [2]Machine Learning Group, Technische Universität Berlin, Berlin, Germany

The scanning probe microscope (SPM) allows nano-objects to be manipulated with single-molecule precision. A critical challenge of this SPM-based technique is to simultaneously manipulate molecules and monitor their configuration. Here, an experimental protocol is developed and evaluated that predicts the molecular configuration based on the physical observables continuously acquired by the SPM. A PTCDA (3,4,9,10-perylene tetracarboxylic dianhydride) molecule on the Ag(111) surface is manipulated to move along a predefined tip trajectory. The measured observables (force gradient) are compared with the results of a DFT trained machine learning model. This work paves the way for the fabrication of a wide variety of nanostructures.

O 17.3 Mon 18:00 P2

**Exploring supramolecular rings by scanning tunneling microscopy** — •Cagri Turan[1], Elie Benchimol[2], Guido Clever[2], and Karina Morgenstern[1] — [1]Physical Chemistry I, Ruhr-Universität Bochum, Germany — [2]Inorganic Chemistry, Technische Universität Dortmund, Germany

Enzymes inspire the design of supramolecular systems, mimicking their catalytic functions for advanced material applications. Among these systems, supramolecular rings and cages are one of the most suitable candidates for mimicking enzyme-like behavior. The use of two different ligands in the heteroleptic supramolecular rings enhances their complexity, enabling the creation of structures that resemble the sophisticated architectures of enzymes. This study reports deposition, self-assembly and inelastic electron tunneling manipulation of PdL2 rings on the Ag(111) surface. The ring molecules were characterized using low-temperature scanning tunneling microscopy in ultra-high vacuum at 7 K. By utilizing an atomic layer injection system, the acetonitrile solvent, used as a solvent during the self-assembly of ligands, will evaporate before the molecules reach the surface, ensuring that only the ring molecules are deposited onto the substrate. Through inelastic electron tunneling manipulation, site-specific manipulations and ligand dissociation processes were explored, offering insights into reaction mechanisms and molecular dynamics on rings on the metallic substrate. The findings contribute to understanding the interaction of supramolecular systems with metal surfaces, enabling advancements in nanoscale functional materials.

O 17.4 Mon 18:00 P2

**Autonomous chemical reactions in scanning tunneling microscopy** — •Nian Wu[1], Peter Liljeroth[1], and Adam S. Foster[1,2] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]WPI Nano Life Science Institute, Kanazawa University, Kanazawa, Japan

Scanning tunneling microscopy (STM) has shown great promise in manipulating atoms or molecules in on-surface molecular synthesis. However, the selection of proper parameters for various manipulations requires extensive explorations and strongly depends on domain knowledge. In particular, the coupling of fragments, as a critical step for polymerizations, necessitates more precise control in rotations and distances. To address this problem, we designed a deep reinforcement learning approach to automate the C-C coupling from Zn(II)-5,15-bis(4-bromo-2,6-dimethylpheny)porphyrin (ZnMe4DPP2.) through learning manipulation parameters in STM, thus enabling the assembly of large polymers based on the building blocks.

O 17.5 Mon 18:00 P2

**Steering intermolecular interaction and ordering of N-heterocyclic carbenes on metal surfaces** — •Duong Tran[1,2], Philipp Wiesener[1,2], Lacheng Liu[1,2], Ankita Das[3], Alex-Cristian Tomut[4], Nikos Doltsinis[4], Frank Glorius[3], Harald Fuchs[1,2], and Harry Mönig[1,2] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]Center for Nanotechnology, Heisenbergstraße 11, 48149 Münster, Germany — [3]Organisch-Chemisches Institut, Universität Münster, Corrensstrasse 40, 48149 Münster, Germany — [4]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

N-Heterocyclic carbenes (NHCs) are established ligands for the chemical and electronic functionalization of surfaces and nanoparticles. Controlling their nucleation and aggregation mechanisms provides valuable opportunities to tune their catalytic- and electro-optical properties. In the present work, we investigate the effect of hydroxyl-side groups on the self-assemblies of IMes on Au(111) and Ag(111) substrates by scanning tunneling microscopy with sub-molecular resolution. Our results are complemented by X-ray photoelectron spectroscopy (XPS) and first-principles calculations. We find that the OH groups can drastically enhance the molecular order, especially on the Ag(111) substrate where extended 2D networks are found. Our findings are essential for robust NHC-based supramolecular networks with tailored properties.

O 17.6 Mon 18:00 P2

**Controlling on-surface chemical reactions through photochemistry** — •Hao Jiang, Yu He, Jiayi Lu, Zhiwen Zhu, and Qiang Sun — Materials Genome Institute, Shanghai University, 200444 Shanghai , China

On-surface synthesis targets extended nanostructures by covalent coupling of organic molecules on surfaces. The most common way to induce reactions of precursor molecules on the surface is by heating, which will however increase the possibility of forming side reactions and lacks selectivity in many cases, thus limiting wider applications of on-surface synthesis. In contrast to the thermally triggered chemistry, photochemistry provides an alternative way to activate molecules. Light has been demonstrated to break certain covalent bonds in a less constructive fashion. Moreover, light has more adjustable parameters such as intensity, wavelength, polarization, etc., to control reactions more finely. Recently, we demonstrated the use of light polarizations to reveal the mechanism of dehalogenation reaction and realized photo induced dechlorination reactionon metal surfaces.

In this poster, we will showcase the wavelength dependence in on-surface synthesis and demonstrate how to harness photochemistry to achieve reaction selectivity in on-surface reactions. Three organic molecules, each with the same functional group, exhibit different chemical reactivities under photon excitation. Our work provides fundamental insights into photoinduced on-surface reactions and illustrates the potential of photochemistry for achieving highly selective and controllable reactions.

O 17.7 Mon 18:00 P2

**Reaction intermediates, organometallic polymers and graphene nanoribbons in on-surface Ullmann-type coupling on coinage metals** — R.S. Koen Houtsma[1], Jeanne van Zuilen[1], Floris van Nyendaal[1], Mihaela Enache[1], and •Meike Stöhr[1,2,3] — [1]University of Groningen, Netherlands — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]University of Applied Sciences of the Grisons, Switzerland

Ullmann-type coupling has been so far the most often employed on-surface reaction for the controlled fabrication of molecular nanoarchitectures in a bottom-up manner. For the case of the prochiral precursor molecule 6,12 dibromochrysene, we compared the influence of substrate material/orientation, annealing temperature and reaction conditions on the reaction outcome. While on Au(111) achiral chevron-type graphene-nanoribbons are formed [1], on Cu(111), Ag(111) [2] and Ag(110) [3] only 1D organometallic polymers were obtained. These 1D polymers are homochiral when Cu(111) was used as substrate whereas they were heterochiral on Ag(111). In the case of Ag(110), their chirality could be even steered via the reaction conditions. With the help of reaction intermediates observed on Ag(111), we obtained key insights into the formation process of the organometallic polymers which is based on the breaking and re-establishing of C-Ag bonds. References: [1] R.S.K. Houtsma et al., Nanoscale Adv. 2022, 4, 3531. [2] R.S.K. Houtsma et al., Adv. Mater. Interfaces 2024, 11, 2300728. [3] R.S.K. Houtsma et al., Commun. Chem. 2024, 7, 51.

O 17.8 Mon 18:00 P2

**LT-STM investigations of subphthalocyanine based vertical molecular rotors on Au (111)** — •Franz Plate[1], Natasha Khera[1], Suchetana Sarkar[1], Soyoung Park[2,3], Ningwei Sun[2,3], Ebru Cihan[1], Dmitry Ryndyk[1,4], 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, TU Dresden, 01069 Dresden Germany — [3]Institute of Applied Polymer Physics (IAPP) TU Hamburg, Kasernenstraße 12, 21073 Hamburg Germany — [4]Professur für Theoretische Chemie, TU Dresden, 01062 Dresden, Germany

We present a vertical rotor based on borsubphthalocyaninchloride (SubPC) platforms adsorbed on Au(111), investigated by low temperature scanning tunneling microscopy. SubPC is a well-investigated molecule which is known to form well-ordered structures, to adsorb flat on the surface and to be highly mobile as a single molecule. The boron atom carries an axial ligand. In this study, SubPC was functionalized with different axial ligands, aiming to create a vertical molecular rotor. The adsorption behavior of SubPC functionalized with azobenzene and 2-methylnaphthalene after thermal evaporation and flash deposition on a cold (5K) surface is presented in high resolution STM images supported by density functional theory (DFT) simulations. In addition, the stabilization through co-deposited pure SubPC and SubPC functionalized with 2-methylnaphthalene is presented.

O 17.9 Mon 18:00 P2

**Adsorption behavior of organoboroxine and organoborthiine based molecules on Au(111)** — •Natasha Khera[1], Franz Plate[1], Karen Marlenne Garcia Alvarez[2], Suchetana Sarkar[1], Andreas Schneemann[2], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Inorganic Chemistry I, TU Dresden, 01069 Dresden, Germany

In this study, we investigate the adsorption behavior of organoboroxine and organoborthiine based molecules on Au (111) surface, employing low temperature scanning tunneling microscopy (LT-STM) and spectroscopy in ultra-high vacuum (UHV) conditions. Organoboroxines provide a model system for constructing Covalent Organic Frameworks (COFs) and are well studied for their applications in catalysis, material science, optoelectronics and energy storage. In contrast, organoborthiines, due to their sulfur mediated interactions, hold promise, making them a compelling area for future research. In this work, a comparative analysis of the adsorption geometries, self-assembled structures and spectroscopic properties of both these molecules is presented.

O 17.10 Mon 18:00 P2

**Chemical activation of a single melamine molecule via isomerization and metalation with a copper atom** — •Karl Rothe[1], Manex Alkorta[2], Nicolas Néel[1], Thomas Frederiksen[3], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau — [2]Centro de Física de Materiales and Fisika Aplikatua Saila, University of the Basque Country, E-20018 Donostia - San Sebastián — [3]Donostia International Physics Center, E-20018 Donostia San Sebastián and IKERBASQUE, Basque Foundation for Science, E-48011 Bilbao

The entire sequence of chemically activating an educt, identifying its reactive site, running a chemical reaction and quantifying the involved forces and energies was performed by means of scanning probe methods. The organic molecule melamine adsorbed on Cu(100) serves as a single-molecule model system for activation via tautomerization and consecutive metalation with a single Cu atom. An atomic force microscope with a CO-decorated tip probes the reactive sites of the isomers at which the subsequent single metal atom transfer is initiated using a Cu-terminated probe. Following the interaction between the mutually approached reaction partners up to the verge of chemical-bond formation enables the access to the force and energy involved in the single-molecule metalation process. Total-energy calculations from density functional theory support the experimental findings and illustrate the structure of the reactants.

Funding by the DFG through KR 2912/18-1 and the BMBF through Forlab is acknowledged.

O 17.11 Mon 18:00 P2

**Metallocorroles: On-Surface Synthesis, Adsorption Geometry, and Electronic Structure** — •Cong Guo, Jan Herritsch, Anastasiya Beliakouskaya, and J. Michael Gottfried — Philipps-Universität Marburg, Fachbereich Chemie, 35043 Marburg, Germany

Tetrapyrrolic macrocycles are widely recognized as fundamental building blocks for interfacial covalent architectures with remarkable stability and atomic precision. Corrole complexes are particularly notable due to their nature as trianionic ligands providing a contracted coordination environment. Herein, we report the on-surface formation and reaction of an octaalkyl-substituted magnesium corrole and an iron triphenylcorrole (FeTPC) on Ag(111). The free-base octaalkyl-corrole forms a well-ordered overlayer . Upon vapor deposition of Mg, the metal atoms incorporate into the corrole cavity, forming Mg-corrole complexes. However, XPS and STM studies show that excessive Mg deposition induces structural deformation and alters the electronic properties of the complex. FeTPC forms different long-range ordered adsorbate structures on Ag(111). During annealing, the degradation of FeTPC occurs, with cyclodehydrogenation leading to the planarization of the ligands, as indicated by XPS and STM. In addition, the ligation of nitric oxide at the Fe center, resulting in significant changes in the electronic properties of the complex, was investigated. These findings highlight the tunability of corrole complexes for tailored applications in catalysis and materials science.

O 17.12 Mon 18:00 P2

**Theoretical investigation of 3,3”-dibromo-p-terphenyl on copper substrate** — •Kevin Eberheim[1], Simone Sanna[1], Michael Dürr[2], and Mohit Jain[2] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]Institut for Applied Physics, Justus-Liebig-University Gießen, Germany

Chemoselectivity is a key parameter for building customized organic nanostructures via bottom-up approaches. Therefore, strategies are needed that allow connecting molecular entities at a specific stage of the assembly process in a chemoselective manner. Studying the mechanisms of such reactions is the key to apply these transformations for the buildup of organic nanostructures on surfaces. Especially, the knowledge about the precise adsorption geometry of intermediates at different stages during the reaction process and their interactions with surface atoms or adatoms is of fundamental importance, since often catalytic processes are involved. With first-principles simulations we can determine the adsorption geometry of the 3,3”-dibromo-p-terphenyl as well as adsorbed mono/diradicals and the halogens. For further comparability with experimental results simulations of Nudged Elastic Band (NEB) have been calculated for transitions between the observed linear chain and ring structures.

## O 18: Poster Focus Session Ultrafast Electron Microscopy at the Space-Time Limit

Time: Monday 18:00–20:00 Location: P2

O 18.1 Mon 18:00 P2

**Extending machine-learning-based band structure reconstruction into the time domain.** — •Mirko Myksa[1], Rui Patrick Xian[1], Vincent Stimper[2], Martin Wolf[1], Ralph Ernstorfer[1], and Laurenz Rettig[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Max Planck Institute for Intelligent Systems, Tübingen, Germany

Reliably extracting the electronic band dispersion from angle-resolved experimental photoemission (ARPES) data poses a challenging task, which often relies on specific line shape models and underlying assumptions, and thereby limiting a systematic and large-scale band structure extraction from volumetric ARPES data. For such purposes, we recently developed a band-structure reconstruction pipeline, including probabilistic machine learning and the associated data processing [1]. This pipeline shows an excellent performance on benchmarks for the reconstruction of three-dimensional photoemission (kx, ky, E) data from various materials. Here, the prospect for extending such analysis towards further dimensions such as pump-probe delay time-resolved ARPES will be discussed.

[1] R.P. Xian, et al., Nat. Comput. Sci. 3, 101 (2023)

O 18.2 Mon 18:00 P2

**Accessing energy- and momentum-dependent electron-phonon coupling from multidimensional photoemission data** — •Hossein Yousofniadarzi, Julian Maklar, Martin Wolf, Ralph Ernstorfer, and Laurenz Rettig — Fritz Haber Institute of the Max Planck Society

Time- and angle-resolved photoemission spectroscopy (trARPES) provides a powerful method for probing ultrafast electron dynamics and their interactions with lattice vibrations. The electron-phonon (e-ph) interaction and its momentum dependence play an important role in many quantum materials, e.g., at the origin of charge-density-wave (CDW) formation. Here, we present an approach based on Fourier analysis, combined with a fitting procedure [1], that allows access to the energy and momentum dependence of the e-ph coupling strength for various coherent phonon modes in several CDW compounds. We discuss how these interactions vary across the Brillouin zone and contribute to the electronic structure modifications characteristic of the CDW phase. This work demonstrates the effectiveness of trARPES as a valuable technique for studying interactions in complex quantum materials.

[1] H. A. Hübener, et al., Phys. Rev. Lett. 125, 136401 (2020)

O 18.3 Mon 18:00 P2

**Machine learning-based denoising and artefact removal for multidimensional photoemission data** — •Joshka Laird, Tommaso Pincelli, and Laurenz Rettig — Fritz haber institute of the Max Planck Society, Berlin, Germany

Angle-Resolved Photoemission Spectroscopy (ARPES) is a powerful tool for investigating the electronic structure of materials. While modern approaches such as momentum microscopy provide rich, multidimensional photoemission data, they pose challenges for achieving high statistics data and good signal-to-noise ratios. Additionally, image distortions such as mesh artefacts often complicate the analysis. Traditional denoising techniques, while effective in specific scenarios, can fail to preserve the fine structural details essential for accurate interpretation.

Here, we present a machine learning-based denoising and artefact removal approach for multidimensional photoemission data. Based on recent results using convolutional neural networks [1], we discuss how to extend such networks to higher dimensions to cope with data e.g. from time-resolved momentum microscopy.

[1] Y. Kim et al., Rev. Sci. Instrum. 92, 073901 (2021)

O 18.4 Mon 18:00 P2

**Towards the Investigation of Spin Systems With Electron Microscopy Tools** — Antonín Jaroš[1,2], Johann Toyfl[1,2], Benjamin Czasch[1,2], •Michael Stanislaus Seifner[1,2], Isobel Claire Bicket[1,2], and Philipp Haslinger[1,2] — [1]Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, Stadionallee 2, 1020 Vienna, Austria — [2]University Service Centre for Transmission Electron Microscopy, TU Wien, Stadionallee 2, 1020 Wien, Austria

Electron spin resonance (ESR) spectroscopy is a method for studying unpaired electrons in various samples with applications in medicine, biology, chemistry, and physics. Typically, the spatial resolution of classical ESR is limited to a few micrometers preventing studying spin systems and their dynamics at the atomic level. To obtain a better understanding of such dynamics, this project aims to develop an ESR setup inside a transmission electron microscope by using the magnetic field created by the objective lens of the microscope to generate energetically separated spin states. A specially designed microcoil integrated into a standard specimen holder allows for exciting spin systems, and various approaches for measuring the resulting resonances are presented. Our results point out potential ways of investigating spin dynamics with sub-nanometer spatial resolution and high temporal resolution. The developed setup will enrich the field of electron microscopy by providing a non-invasive tool to investigate spin systems as well as certain electron beam-induced sample damage.

O 18.5 Mon 18:00 P2

**Characterization and Improvement of the Electron Beam Stability and the Measurement Noise in Ultrafast Low-Energy Electron Microscopy** — •Ole Böttger[1,2], Johannes Otto[1,2,3], Leon Brauns[1,2], and Claus Ropers[1,2,3] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany — [3]Max Planck School of Photonics

Ultrafast Low Energy Electron Microscopy (ULEEM) promises to uncover real-space dynamics on surfaces with few-picosecond temporal and nanometer spatial resolutions. Our group is currently developing such an instrument and has obtained first promising results [1]. The extended measurement durations required in this scheme require a high degree of long-term stability of the system. Here, we present results of energy, beam position and intensity stability measurements under various operating conditions, applied to both the laser pump and electron probe beam used. Moreover, we show results of state-of-the-art drift correction algorithms [2] applied to first ULEEM data [1].

[1] J. Otto et al., in preparation (2024).

[2] T. A. de Jong et al., Ultramicroscopy 213, 112913 (2020).

O 18.6 Mon 18:00 P2

**Monochromatization of Electron Beams with Spatially and Temporally Modulated Optical Fields** — •Neli Laštovičková Streshkova[1], Petr Koutenský[1], Tomáš Novotný[2], and Martin Kozák[1] — [1]Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, CZ-121 16 Prague, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, Prague CZ-12116, Czech Republic

Inelastic interaction between coherent light and free electrons is a powerful tool for modulating electron wave packets, typically resulting in periodic sidebands in the electron energy spectra. We present a novel approach leveraging a time-dependent frequency modulation of light fields to achieve spectral squeezing and monochromatization of free electron pulses. This method compensates for the energy chirp inherent to dispersive propagation in electron sources like TEMs and SEMs, where finite coherence lengths lead to broadened energy spectra. By correcting the chirped wave packet in the energy-time domain through inelastic interaction with tailored optical fields, we enable significant spectral narrowing. Up to 26% of the electron distribution is concentrated within a narrowed energy band, achieving spectral compression by a factor of five. This advancement has implications for high-resolution quantum sensing and electron-based spectroscopy, addressing a critical need for low-loss electron monochromatization.

O 18.7 Mon 18:00 P2

**Spatio-Temporal Electron Propagation Dynamics in Au/Fe/MgO(001) in Nonequilibrium** — Markus Heckschen[1], Yasin Beyazit[1], Elaheh Shomali[1], Florian Denizer[1], J. Jayabalan[1], Ping Zhou[1], Detlef Diesing[2], Markus Gruner[1], Rossitza Pentcheva[1], Axel Lorke[1], Björn Sothmann[1], and •Uwe Bovensiepen[1] — [1]University of Duisburg-Essen, Faculty of Physics and CENIDE, 47048 Duisburg — [2]University of Duisburg-Essen, Faculty of Chemistry, 45141 Essen

Since the mean free path of hot electrons is only a few nanometer, insights into the spatio-temporal electron dynamics are desired for the analysis of ultrafast microscopy. We determine the energy-dependent electron propagation time through epitaxial Au/Fe(001) as a function of Au layer thickness [1] by femtosecond time-resolved two-photon photoemission spectroscopy at energies 0.5-2.0 eV above $E_\mathrm{F}$. By combining real-time time-dependent density functional theory and microscopic electron transport simulations we identify ballistic transport of minority electrons of the optically excited electron population. At lower energy, superdiffusive transport with 1-4 scattering events dominates. The effective electron velocity accelerates from 0.3 to 1 nm/fs with an increase in the Au layer thickness from 10 to 100 nm which is explained by electron transport that becomes preferentially aligned with the interface normal for thicker Au layers. On this basis the electron momentum or energy can be selected by the choice of the propagation layer thickness. We acknowledge funding by the DFG through SFB 1242. [1] Heckschen et al., PRX ENERGY **2**, 043009 (2023).

## O 19: Poster Surface Magnetism

Time: Monday 18:00–20:00 Location: P2

O 19.1 Mon 18:00 P2

**Studying Higher-Order Interaction Driven Non-Coplanar Spin Structures Using SP-STM** — •Arved Heilmann, Roland Wiesendanger, and Kirsten von Bergmann — Universität Hamburg, Germany

Complex magnetic order arises from competing interactions between magnetic moments. Higher-order interactions (HOI), involving more than two spins, can lead to three-dimensional magnetic configurations known as multi-Q states. Spin-polarized scanning tunneling microscopy (SP-STM) is a powerful tool for studying these systems, enabling real-space imaging of atomic-scale magnetic structures. HOI-driven hexagonal 3Q states have been observed at the atomic and nanoscale in Rh/Mn/Re(0001) and Fe/Rh/Ir(111), respectively [1,2].

To identify further HOI-driven magnetic states, we investigate other systems with Mn/Rh and Fe/Rh interfaces grown on Re(0001). Our findings reveal distinct spin structures that depend on the layer sequence of the pseudomorphic layers. Mn monolayers grown on single or double Rh layers form the Néel state, while Mn grown directly onto the substrate exhibits a non-coplanar 3Q state [3]. For Fe, deposition on two Rh layers results in a distorted quasi-hexagonal magnetic lattice, contrasting with the substrate's ideal hexagonal symmetry. This two-dimensional modulation of the spin texture suggests it also arises from HOI.

[1] F. Nickel, et al., Phys. Rev. B **108**, L180411 (2023).
[2] M. Gutzeit, et al., Nat. Commun. **13**, 5764 (2022).
[3] J. Spethmann, et al, Phys. Rev. Lett. **124**, 227203 (2020).

O 19.2 Mon 18:00 P2

**Design of a STM/ nc-AFM head to quantify the magnetic exchange interaction between individual atoms** — •Karoline Oetker, Zhengyuan Liu, Henning von Allwörden, Alexander A. Khajetoorians, and Nadine Hauptmann — IMM, Radboud University, Nijmegen, The Netherlands

STM methods are highly powerful tools to quantify the magnetic coupling between single adatoms and with the atom at the tip [1,2]. These current-based methods prohibit to probe the atomic-scale magnetic properties of adatoms on thick insulating layers. However, it was shown that thicker insulating layers with a 4-fold symmetry, as MgO, can prohibit single-electron induced ground state transitions and only allow higher-order excitation processes, which stabilizes the magnetic moment of the adatom [3]. Therefore, a force-based method, such as magnetic exchange force microscopy (MExFM), is a promising tool to quantify the different magnetic coupling mechanisms between individual adatoms on thick insulating layers. We present the design of a 1K STM/nc-AFM setup dedicated for MExFM measurements in magnetic fields up to 9T, based on the tuning fork design. Our goal is to quantify the different distance-dependent magnetic interactions between different magnetic atoms, e.g. 3d and 4f elements. We will utilize functionalized tips with different magnetic atoms, to probe the distance-dependent magnetic exchange force between the tip and adatoms on thick insulating layers. 1.Meier, F. et al., Science 320, 82-86 (2008), 2. Baumann, S. et al., Science 350, 417-420 (2015). 3.Donati, F. et al., Science 352, 318-321 (2016).

## O 20: Poster Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale

Time: Monday 18:00–20:00 Location: P2

O 20.1 Mon 18:00 P2

**Generation of single cycle terahertz pulses for a THz-STM and improvement of the current measurement noise** — •Paul Wiechers, Christian Lotze, Florian Faaber, Vibhuti Rai, and Katharina J. Franke — Freie Universität Berlin, Fachbereich Physik,Arnimallee 14, 14195 Berlin, Germany

Terahertz Scanning Tunneling Microscopy (THz-STM) aims to combine the atomic spatial resolution of STM with the sub-picosecond time resolution commonly achieved through optical pump-probe techniques.

We generate single-cycle terahertz pulses by optical rectification and short optical pulses of various wavelengths. Particular care is taken to minimize pointing deviations of the beams, ensuring proper focusing in the STM junction, even under varying beam delay positions.

In a THz-STM experiment, the measured quantity is the low-bandwidth tunneling current. The THz-induced part of that current, due to the low duty cycle ($\sim 10^{-5}$) of the THz pulses, is very small. Thus, a thorough understanding of the limiting noise sources in the measurement is important. Here, we characterize a cryogenic low-noise ammeter and increase its prohibitively low bandwidth by more than two orders of magnitude.

O 20.2 Mon 18:00 P2

**Local excitation of coherent phonons in 2H-MoTe$_2$ by THz driven scanning tunnelling microscope** — Vibhuti Rai, Junyoung Sim, •Florian Faaber, Sergey Trishin, Nils Bogdanoff, Tom Seifert, Tobias Kampfrath, Christian Lotze, and Katharina J. Franke — Freie Universität Berlin, Department of Physics, Arnimallee 14,14195 Berlin, Germany

The coupling of THz pulses into a scanning tunnelling microscope has emerged as a unique technique to achieve picosecond time resolution while maintaining sub nanometer spatial resolution [1,2]. By delaying one THz pulse with respect to the other while recording the current rectified by the two pulses, a pump-probe scheme can be realized [3]. In this work, we use this scheme to investigate the quasi 2D semiconducting transition metal dichalcogenide (TMD) 2H-MoTe$_2$ at 7K in ultra-high vacuum and find a large oscillatory rectified current that is slowly decaying over 50 ps. We attribute these oscillations to the excitation of coherent phonons and discuss the effect of defects and DC bias voltage on the excited modes.

[1] Cocker, et al., Nature Photonics 7, 620*625 (2013)
[2] V. Jelic et al., Nature Physics 13, 591 (2017)
[3] T. L. Cocker et al., Nature 539, 263 (2016)

O 20.3 Mon 18:00 P2

**Charging of atomic defects in 2H-MoTe$_2$ under infrared illumination** — •Friedemann Lohss, Florian Faaber, Vibhuti Rai, Junyoung Sim, Christian Lotze, and Katharina J. Franke — Freie Universität Berlin, Department of Physics, Arnimallee 14,14195 Berlin, Germany

The electronic properties of semiconductors are heavily shaped by the concentration and type of defects present in the material. The sub-nanometer resolution of scanning tunneling microscopy (STM) allows to locally probe such defects. Here we characterize the response of the semiconductor 2H-MoTe$_2$ to infrared illumination in an STM at cryogenic temperature. We observe the formation of disc-shaped regions of increased conductivity around some local defects, likely stemming from charging and tip-induced band bending. We characterize the different defect states occuring in this material.

O 20.4 Mon 18:00 P2

**Two-Color Pump-Probe STM of Coherent Phonon Dynamics in Ultrathin ZnO/Ag(111)** — •Henrik Wiedenhaupt[1], Shuyi Liu[2], Akitoshi Shiotari[1], Adnan Hammud[1], Daniel Wegkamp[1], Martin Wolf[1], Takashi Kumagai[3], and Melanie Müller[1] — [1]Fritz Haber Institute of MPG, Berlin, Germany. — [2]Huazhong University of Science & Technology, Wuhan, China. — [3]Institute for Molecular Science, Okazaki, Japan.

We use photon-assisted ultrafast scanning tunneling microscopy (ph-USTM) to study coherent phonon (CP) dynamics in optically excited ZnO/Ag(111). In recent work, we have shown that resonant single-color ph-USTM enables CP spectroscopy on 3ML-ZnO/Ag(111) with nanometer spatial resolution [1], where the optical resonance between an interface state (IS) and the ZnO conduction band edge (CBE) appears to play an important role, as also observed in tip-enhanced Raman spectroscopy (TERS) [2]. However, the detailed mechanisms by which the CPs modulate the photocurrent and of their local excitation remain unclear. To gain further insight, we implement two-color ph-USTM for the selective on- and off-resonant ultrafast excitation of the IS-CBE transition on 2ML-ZnO and 3ML-ZnO. Besides demonstrating local CP spectroscopy also on 2ML-ZnO, our results show that CPs can also be excited off-resonantly, while optically resonant photon-assisted tunneling seems to be more crucial for local CP detection via ph-USTM. We explain our observations by phonon-induced transient changes in the local dielectric response. [1] S. Liu et al., Sci. Adv. 8, 42, eabq5682 (2022) [2] S. Liu et al., Nano Lett. 19, 8, 5725 (2019)

O 20.5 Mon 18:00 P2

**Plasmonic STM-luminescence driven by a high-power spintronic THz emitter** — •Alkisti Vaitsi, Luis Enrique Parra López, Vivien Sleziona, Martin Wolf, and Melanie Müller — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

We demonstrate THz-induced STM-luminescence (THz-STML) from a plasmonic tunnel junction driven by broadband single-cycle THz pulses generated from a high-power rotating spintronic THz emitter (STE). By measuring the dependence of the plasmonic luminescence on the static STM bias and the THz-STM bias, we aim for a purely data-driven approach to calibrate the THz peak bias via reconstruction of the THz-STML spectra from the static reference STML spectra. Our results proof the capability of the rotating STE to generate several Volts peak THz bias in a metallic STM junction and pave the way for future time-resolved gating of STM-luminescence from excitonic quantum emitters.

[1] Kimura et al., ACS Photonics 8, 4, 982-987 (2021)

[2] Vaitsi et al., Appl. Phys. Lett. 125, 071107 (2024)

O 20.6 Mon 18:00 P2

**Scanning Quantum Microscopy for Emergent Phases of Matter** — •Ruoming Peng[1], Sreehari Jayaram[1], Malik Lenger[1], King Cho Wong[1], Xuankai Zhou[1], Yan Tug Kong[1], and Joerg Wrachtrup[1,2] — [1]3. Physikalisches Institut, University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Scanning quantum microscopy using NV centers in diamond enables direct visualization of condensed matter phenomena. Applying this technique, we uncover the emergence of a super-Moiré magnetic texture in twisted double bilayer CrI3, distinct from the geometric Moiré periodicity at small twist angles. Additionally, we investigate vortex dynamics in thin-layer 2H-NbSe2, revealing vortex melting behaviors during different thermal cycling and unconventional magnetic noise arising from the vortex dynamics. Our findings highlight the strong capability of scanning quantum microscopy to unravel nanoscale magnetic interactions and dynamic phases in 2D materials.

O 20.7 Mon 18:00 P2

**A theoretical perspective on electroluminescence, photoluminescence and photocurrent generation in a scanning tunneling microscope** — •Tomáš Neuman[1], Sofia Canola[1], Rodrigo Ferreira[1], Anna Roslawska[2], Katharina Kaiser[3], Alex Boeglin[4], Andrei Borisov[5], Guillaume Schull[4], and Martin Švec[1] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czechia — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Georg-August-Universität Göttingen, Göttingen, Germany — [4]Université de Strasbourg, IPCMS, CNRS, UMR 7504, Strasbourg, France — [5]Université Paris-Saclay, Institut des Sciences Moléculaires d'Orsay, CNRS, UMR 8214, Orsay, France

The phenomena occurring in a scanning tunneling microscope (STM) that lead to the generation of light or are triggered by light (STM+light, STM+L), including the STM-induced luminescence and photocurrent generation in single molecules, allowed for studying excited states of molecules in a STM. As the underlying principles of these phenomena involve electron tunneling, plasmon-enhanced optical absorption and spontaneous emission, and vibronic effects, interpreting these STM+L experiments hinges on the development of theoretical models. I will show such modelling strategies and showcase its application to recent experiments. In particular, I will focus on the theory of mapping of orbitals of a multireference excited state of a small molecule (perylene tetracarboxylic dianhydride - PTCDA) via photocurrent generation, whose explanation requires all the mentioned ingredients.

O 20.8 Mon 18:00 P2

**Neutral Exciton-Libron Coupling via Resonant Energy Transfer in Single Molecules** — •Thiago G. L. Brito[1], Klaus Kuhnke[1], Klaus Kern[1,2], and Anna Rosławska[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The optical properties of single molecules can vary depending on their environment. In some surroundings, vibrations due to frustrated rotations (librations) may occur if the molecules feature some rotational freedom. In this study, we provide evidence of coupling between neutral excitons and libration modes (librons). We observed this coupling through light emission resulting from resonant energy transfer (RET). We measured neutral and charged exciton emissions in isolated zinc phthalocyanine (ZnPc) and ZnPc-platinum phthalocyanine (PtPc) assemblies deposited on NaCl/Ag(111) using scanning tunneling microscopy induced luminescence (STML). For isolated ZnPc, we observed a broad peak from the neutral exciton and exciton-libron coupling for the charged exciton. In contrast, in ZnPc-PtPc structures, we found libronic signatures in the neutral emission of ZnPc when excited via RET from PtPc. This study is providing deeper insights into exciton-libron dynamics in single molecules.

O 20.9 Mon 18:00 P2

**Mapping adsorbed states of iron(II) phthalocyanine on Ag surfaces by plasmon-enhanced Raman spectroscopy** — Borja Cirera[1], •Rodrigo Cezar de Campos Ferreira[2,3], Amandeep Sagwal[2], Jiří Doležal[3], Martin Švec[2,3], and Pablo Merino[1] — [1]Instituto de Ciencia de Materiales de Madrid, Spain — [2]Institute of Physics, Czech Academy of Sciences, Czech Republic — [3]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Czech Republic

The high spatial confinement of a plasmonic field in LT-SPM has become a valuable tool for near-field spectroscopies. Among the techniques, Raman scattering enables chemical identification, investigation of relations between adsorption geometry and vibrational fingerprints in real space at single-molecule level.[1,2] Here we studied different adsorption configurations of iron(II) phthalocyanines (FePc) on Ag(110) and Ag(111) crystal surfaces. Real-space mapping reveals the appearance of shifted Raman states when adsorbed in specific geometries. Results and simulations suggest that the breaking in symmetry with respect to the main crystallographic directions of the substrates are the leading reason for this phenomenon. [1] Y. Zhang et. al. Nature 498, 82-86 (2013). [2] R. Zhang et. al. National Science Review, Volume 6, 2019, 1169-1175.

O 20.10 Mon 18:00 P2

**Investigations of the plasmon excitation of C60 multilayers on Au(111) using STM induced luminescence** — •Andreas Reutter, Yannis Hilgers, Markus Etzkorn, and Uta Schlickum — Institute of Applied Physics - LENA, TU Braunschweig

In recent years, Scanning Tunneling Microscopy induced luminescence (STML) has gathered great interest, as it allows to investigate optical properties in addition to normal STM measurements, both with atomic spatial resolution. Since its development, the main challenge of this method is to obtain reasonable photon intensities.

We succeeded in building a setup with a greatly increased detection efficiency by using a parabolic mirror inside the STM, that covers 75% of the upper hemisphere.

Here, we present STML measurements of surface plasmons on C60 on Au(111) as a model system for the effects of an organic semiconductor on a metal surface [1]. We will present conductance and optical spectroscopy measurements as well as photon yields for different number fo C60 layers and different applied voltages.

[1] Große, Christoph; Merino, Pablo; Rosławska, Anna; Gunnarsson, Olle; Kuhnke, Klaus; Kern, Klaus; ACS Nano, 11, 1230 (2017).

O 20.11 Mon 18:00 P2

**Resonant energy transfer as a function of distance between metal-phthalocyanine molecules** — •Roel Burgwal, Nikhil Seeja Sivakumar, Joëlle J. A. Schrijer, Alexander A. Khajetoorians, and Daniel Wegner — Institute for Molecules and Materials, Radboud University, 6500 GL Nijmegen, The Netherlands

Resonant transfer of energy (RET) between molecules is a process ubiquitous in nature that also has interesting technological applications. The rate of RET decreases as the molecules involved are spaced further apart, with the distance dependence determined by the exact mechanism responsible for energy transfer. Two possible mechanisms are electrodynamical Förster energy transfer (FRET) and the electron tunneling-based Dexter energy transfer (DET). Recent advances in scanning tunneling microscope-induced luminescence (STML) have made it possible to observe energy transfer between single molecules and to control the spacing between these with sub-nanometer precision. So far, STML measurements of RET distance dependence resemble more the exponential behavior of DET, in contrast with the commonly assumed FRET mechanism. However, it has been proposed this apparent behavior may be a plasmonic effect arising from the varying distance between STML-tip and acceptor molecule. Here, we study RET between different metal-phthalocyanine molecules while elucidating the role of the plasmon through complementary measurements.

## O 21: Poster Heterogeneous Catalysis

Time: Monday 18:00–20:00 Location: P2

O 21.1 Mon 18:00 P2

**Disentangling Transport and Kinetics in Complex Reaction Chambers by Novel Reduced-Order Modeling Approaches** — •Tobias Hülser[1], Maryke Kouyate[1], Uzair Qureshi[2], Daniel Runge[3], Georg Brösigke[2], Christian Merdon[3], Jürgen Fuhrmann[3], Karsten Reuter[1], Christoph Scheurer[1], and Sebastian Matera[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Technische Unviversität Berlin — [3]Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin

*Operando* catalytic characterization chambers are governed by mass transport interplaying with highly-nonlinear chemical kinetics, which needs to be accounted for by corresponding coupled simulations. Often, these chambers can not be modelled with established reactor models, instead requiring high-cost Computational Fluid Dynamics simulations. We have developed reduced-order methods which disentangle the computational treatment for transport and kinetics into an offline (OffPh) and online phase (OnPh). In the OffPh, we determine a suitable solution space of the transport operator, which is independent of the employed kinetic model and therefore reusable. In the OnPh, the solution from this space is determined from the balance of transport and kinetics at the catalytic surfaces. This drastically reduces the costs as the OffPh is a linear problem and, particularly, the nonlinear online phase typically involves only very few degrees of freedom. We demonstrate this idea on mesoscale core-shell particles, an asymptotic expansion for small catalyst samples and a quasi-exact reduced basis strategy for general problem settings.

O 21.2 Mon 18:00 P2

**Bayesian Inference of Kinetic Models of Heterogeneous Catalysis by Normalizing Flows** — •Andreas Panagiotopoulos[1], Javed Mudassar[2], Jens-Uwe Repke[2], Georg Brösigke[2], and Sebastian Matera[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Technical University Berlin

Estimating kinetic parameters is typically done by classical fitting a model to experimental reactor data, which, however, suffers from a number of fundamental problems like ill-posedness, multiple possible solutions and the lack of reliable uncertainty estimates. By reformulating the problem in a probabilistic language, Bayesian inference cures these problems, but also requires to sample from a high-dimension probability distribution. Because of their high non-linearity and sensitivity, this becomes challenging for kinetic models and established sampling approaches become inefficient. We investigate Normalizing Flows in conjunction with Quasi Monte Carlo sampling to address this problem. In this approach, a bijective nonlinear parameter transformation is sequentially learned such that a uniform sampling from the transformed parameters leads to a good importance sampler of the Bayesian posterior. We investigate the performance of the proposed approach on an empirical model for methanol synthesis on Cu based catalysts using synthetic and experimental data.

O 21.3 Mon 18:00 P2

**Model Catalytic Studies on the Thermal Dehydrogenation of the Benzaldehyde/Cyclohexylmethanol LOHC System on Pt(111)** — •Marius Steinmetz[1], Valentin Schwaab[1,2], Felix Hemauer[1,2], Eva Marie Freiberger[2], Natalie J. Waleska-Wellnhofer[2], Hans-Peter Steinrück[2], and Christian Papp[1] — [1]Angewandte Physikalische Chemie, Freie Universität Berlin (FU Berlin), Arnimallee 22, 14195 Berlin, Germany — [2]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Egerlandstr. 3, 91058 Erlangen, Germany

We investigated the dehydrogenation reaction and the thermal decomposition of the liquid organic hydrogen carrier (LOHC) pair benzaldehyde/cyclohexylmethanol on a Pt(111) model catalyst via temperature-programmed desorption experiments and synchrotron radiation photoelectron spectroscopy. The LOHC pair has a hydrogen storage capacity of 7.0 mass%, stored in a cyclohexyl ring and a primary alcohol group. We observed a stepwise dehydrogenation mechanism, starting with the dehydrogenation of the alcohol group, followed by the dehydrogenation of the cyclohexyl ring. We also observed different dehydrogenation behaviors for low and high coverages, probably caused by steric hindrance for high coverages. Even though the LOHC pair achieves high hydrogen storage capacity, early decomposition at low temperatures between 250 and 350K limits the use of the molecule pair as a reversible hydrogen carrier.

O 21.4 Mon 18:00 P2

**Size-selected metal nanoparticles on tungsten: influence of the deposition angle** — •Sumanasa Begur Prakash and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

Metal nanoclusters and nanoparticles, especially those composed of iron (Fe), nickel (Ni), and their alloys, are fascinating due to their unique electronic and magnetic properties which vary significantly with particle size. This feature makes them not only interesting for fundamental research but also highly promising for advanced technologies including catalysis, magnetic storage, and sensing. However, interaction with the substrate during and after deposition significantly influences the particle's properties.

Our contribution is focused on size-selected Fe, Ni, and Fe-Ni alloy nanoparticles which are deposited on a W (110) substrate. Using a magnetron sputter source (Haberland-type) we vary the deposition angle to understand how this parameter influences the particle size, structure, and overall distribution of nanoparticles on the substrate surface. This approach allows us to probe the relationship between deposition conditions and particle characteristics. The size and structural properties are investigated by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) under ultra-high vacuum (UHV) conditions.

O 21.5 Mon 18:00 P2

**Optimized BiVO4/g-C3N4 Heterojunctions for Efficient Photocatalytic Green Ammonia Production** — •Susana D. Rojas[1], Nicolás A. Soto[1], Pablo E. Salinas[1], Daniel Saavedra[2], Marcelo A. Cisternas[1], and Ulrich G. Volkmann[2] — [1]Escuela de Ingeniería Industrial, Universidad de Valparaíso, Santiago, Chile — [2]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile

BiVO4 nanostructures were synthesized via a hydrothermal method, and g-C3N4 nanosheets by urea pyrolysis. The materials were characterized using Fourier transform IR spectroscopy (FTIR), UV-Vis and X-ray photoelectron spectroscopy, X-ray diffraction, and scanning electron microscopy to confirm their chemical and morphological structures. Photocatalytic ammonia production was evaluated in a cylindrical reactor with a Xenon discharge lamp, using an aqueous catalyst dispersion under magnetic stirring and a nitrogen flow at atmospheric pressure. Ammonia production was analyzed via the Nessler method with ammonium chloride (NH4Cl) calibration curves for the aqueous phase and in situ FTIR spectroscopy with a 16 m optical path gas cell for the gas phase [1, 2]. This work advances the understanding of photocatalytic processes for sustainable ammonia production and the development of efficient, eco-friendly methods for synthesizing this essential compound. Acknowledgements: ANID project SIA77210032 (SR, MC), UVA22991 (SR, MC), ANID Fellowship (DS), and Puente UC 2024-25 (UV). Ref.: [1] P. Huang, et al., Nature Comm. 13, 7908 (2022). [2] S.Z. Andersen, et al., Nature 570, 7762, 504-508 (2022).

O 21.6 Mon 18:00 P2

**Tuning the ceria island orientation: from (111) to (100)-oriented islands** — •Maja Atlas, Raquel Sanchez-Barquilla, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany

Inverse catalysis systems, where the reducible oxide is anchored on the metallic support, have shown a better performance compared with its traditional counterparts due to the strong metal support interaction. Among catalytic materials, ceria ($CeO_2$) is used in a wide range of applications, due to its oxygen storage and redox properties. In particular, the catalytic activity of Cu(111) can be substantially enhanced when depositing $CeO_x$ on top, achieving direct methanol production from $CO_2$. In situ near ambient pressure X-ray photoemission spectroscopy (NAP-XPS) measurements have shown that the activated $CO_2$ molecule is stabilized by $Ce^{3+}$ sites during the reaction. Moreover, epitaxially grown $CeO_2$ islands can have two different orientations on Cu(111): the (111)-oriented islands appear first and with lower oxygen pressure, while the (100)-oriented phase can be enhanced by increasing the oxygen exposure. Here, we present a structural and chemical study of the ceria islands growth as a function of temperature, oxygen pressure and deposition rate. By varying these parameters, we can study the relation between the phase and the $Ce^{3+}/Ce^{4+}$ ratio, using XPS, low energy electron diffraction (LEED) and scanning tunneling microscopy (STM).

O 21.7 Mon 18:00 P2

**Structure and chemical properties of Pt clusters and particles deposited on CeO$_2$(111)** — •Shuang Chen, Zairan Yu, Alexei Nefedov, Christof Wöll, and Yuemin Wang — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

CeO$_2$-supported Pt nanoparticles are of significant technological interest due to their unique catalytic properties and wide range of applications in numerous chemical reactions. However, the catalytic performance of various Pt species remains a highly debated topic. This arises primarily from the complexity of Pt/CeO$_2$ powder catalysts and the scarcity of accurate reference data obtained from well-defined model systems. Here, we report systematic IR reflection absorption spectroscopic (IRRAS) investigations of Pt deposited on oxidized CeO$_2$(111) single-crystal surfaces. By employing polarization-resolved IRRAS with CO as a probe molecule and grazing-emission XPS, we were able to track the structural and electronic evolution of Pt on CeO$_2$(111) as a function of the deposition amount. Various Pt species, ranging from single atoms to small clusters and large particles, were identified. Our results provide solid evidence of strong electronic interactions between Pt and the ceria substrate, offering profound insights into the dynamic behavior of Pt clusters under different conditions. This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) -Project-ID 426888090- SFB 1441.

O 21.8 Mon 18:00 P2

**Photoelectrochemical nitrate reduction by copper oxide-based semiconductors** — •Jasmin A. Zitzmann[1,2], Maximilian Christis[1,2], Saswati Santra[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

The photoelectrochemical nitrate reduction reaction (PEC-NO$_3$RR) offers a route to ambient ammonia (NH$_3$) synthesis and recycling of $NO_3^-$ pollutants. Copper oxide-based semiconductors, such as Cu$_2$O, CuO and CuBi$_2$O$_4$ exhibit suitable band energetics to drive this reaction. While Cu$_2$O is reported for PEC-NO$_3$RR, further studies are required to optimize reaction conditions and minimize photocorrosion. With this aim, the PEC-NO$_3$RR performance characteristics of Cu$_2$O, CuO and CuBi$_2$O$_4$ are investigated in alkaline and neutral aqueous electrolytes. The dominant reaction product observed is nitrite ($NO_2^-$) with Cu$_2$O producing the highest yields. In addition, NH$_3$ is generated by Cu$_2$O, with an increase in selectivity at lower potentials. Photocorrosion is most pronounced for CuO, whereas CuBi$_2$O$_4$ shows the most consistent PEC stability. Our findings indicate the potential-dependent PEC-NO$_3$RR product selectivity, with further research necessary to optimize the electrochemical conditions to improve PEC-NO$_3$RR stability and NH$_3$ yield using these promising copper oxide-based semiconductors.

## O 22: Poster Surface Reactions

Time: Monday 18:00–20:00 Location: P2

O 22.1 Mon 18:00 P2

**TRACE/TRIADE: A setup to investigate tritium accumulation of solids** — •Marie-Christine Schäfer, Dominic Batzler, James Braun, Robin Grössle, Philipp Haag, Elizabeth Paine, Marco Röllig, Marius Schaufelberger, and Kerstin Trost — Tritium Laboratory Karlsruhe, Eggenstein-Leopoldshafen, Germany

In the context of the KArlsruhe TRItium Neutrino experiment (KATRIN), sufficient knowledge of the accumulation of tritium on surfaces is crucial for minimising systematic effects, thus optimising the experiment. On a bigger scale, the understanding of these specific tritium gas-surface interactions is relevant when it comes to fusion reactors and their fuel cycles. In search of materials with small tritium memory effects, the Tritium Activity Chamber Experiment (TRACE) at Tritium Laboratory Karlsruhe (TLK) provides the possibility of exposing solid samples to high purity tritium gas while monitoring the near-surface activity via beta-induced X-ray-spectrometry (BIXS). Similarly, the TRItium Adsorption Desorption Experiment (TRIADE) also measures the tritium accumulation via the BIXS method but is being upgraded to additionally provide the option of studying adsorption and desorption processes at temperatures down to 100 K. For this, a newly designed sample holder is currently being tested. Besides investigating the tritium accumulating properties of different materials, the compatibility with UV/ozone in the context of decontaminating the surfaces is also of relevance. For this, experiments with an additional setup are set to be conducted in the near future. This contribution will present the TRACE/TRIADE setups as well as their planned modifications.

O 22.2 Mon 18:00 P2

**Exploring TiO$_2$-water-interfaces with AIMD and Machine Learning Force Fields** — •Johannes Laurenz Wolf, Christian Dressler, and Malte Grunert — Technische Universität Ilmenau, Department of Physics, 98693 Ilmenau, Germany

Titanium dioxide (Ti$O_2$) is a pivotal material in photocatalysis, particularly for water splitting applications in artificial leaves. In this study, we employ ab initio molecular dynamics (AIMD) and machine learning force fields (MLFF) within the MACE framework to investigate systems comprising, Ti$O_2$ layers in different crystalline phases on indium phosphide (InP) and water. A central focus is placed on the structural and dynamic properties of the Ti$O_2$-water interface.

To enhance our understanding of interfacial interactions, we introduce nanoscale pinholes into the Ti$O_2$ layer, exploring their impact on water adsorption and hydrogen bonding dynamics. AIMD simulations provide atomic-scale insights, while MLFF extends these analyses to longer time scales, enabling a comprehensive investigation of adsorption mechanisms, titanium coordination, and local surface distortions.

O 22.3 Mon 18:00 P2

**Investigation of the water-GaN($10\bar{1}0$) and water-GaN(0001) interface by ab initio molecular dynamics simulations** — •Marius Otto, Christian Dressler, Fabian Ullmann, and Stefan Krischok — Technische Universität Ilmenau

We have performed ab initio molecular dynamics simulations to investigate the dissociative adsorption of water at the water-GaN($10\bar{1}0$) and water-GaN(0001) interfaces. Our results confirm that water undergoes dissociative adsorption on both surfaces, with notable differences in the protonation states of the adsorbed oxygen species. On the non-polar GaN($10\bar{1}0$) surface, Ga atoms are exclusively coordinated by hydroxyl (OH) groups, whereas the polar GaN(0001) surface shows a mixed coverage of hydroxyl (OH) and water ($H_2O$) species. The dissociation of water is significantly more pronounced on the GaN($10\bar{1}0$) surface due to the availability of distinct adsorption sites for both hydrogen and hydroxyl groups. In contrast, on the GaN(0001) surface, steric shielding of the adsorption sites inhibits water dissociation, resulting in reduced reactivity. In addition, we have also compared our simulations to XPS and UPS measurements.

O 22.4 Mon 18:00 P2

**kinetics and thermodynamics of dehalogenation on metal surfaces** — •Yu He[1], Hao Jiang[1], Zhiwen Zhu[1], Juan Xiang[1], Jinyang Xu[2,3,4], Zhaofeng Liang[2], Lei Xie[2], Fei Song[2], and Qiang Sun[1] — [1]Materials Genome Institute of Shanghai University,Shanghai,China — [2]Shanghai Synchrotron Radiation Facility, Shanghai Advanced Research Institute, Chinese Academy of Sciences, Shanghai,China — [3]Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai,China — [4]University of Chinese Academy of Sciences, Beijing,China

In the field of on-surface synthesis, dehalogenative aryl-aryl coupling has become the key strategy for the fabrication of covalently bonded carbon-based nanomaterials. However, studies on the kinetics and thermodynamics of these reactions are still scarce. Also, most of the works focus on debromination while overlooking the dechlorination reaction which is a fundamental reaction with significant implications for environmental protection and sustainable chemistry. Here, we combined synchrotron-based x-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM) to study the dehalogenative polymerization reactions of chlorinated and brominated aromatic hydrocarbons on the Au(111) surface. We resort to high-resolution surface-sensitive techniques to identify the reactants and products as well as the important reaction intermediates. Using the fast XPS, we are able to extract the kinetic curves of the reactions and obtain detailed insight into the reaction process. Our research deepens the understanding of the reaction mechanism.

O 22.5 Mon 18:00 P2

**Self-assembly and reactions of benzonitriles on metal surfaces** — •Anran Bao[1] and Wenshao Yang[2] — [1]Physikalische Chemie I, Ruhr-Universität Bochum, Bochum, Germany — [2]Hangzhou Institution of Advanced Studies, Hangzhou,China

Surface synthesis enables innovative material design, with the self-assembly of organic molecules on metal surfaces. Among on-surface reactions, the Ullmann coupling is significant. Notably, despite the considerable differences in the chemical structures of cyanides and halogen atoms, they exhibit similarities in organic reactions. This provides a new perspective on surface synthesis and possibilities for synthesizing novel nanomaterials. This study focuses on the unique self-assembly and chain formation of benzonitrile derivatives, particularly iso-phthalonitrile (IPN), tere-phthalonitrile (TPN) and ortho-phthalonitrile (OPN), on the Co(0001) surface. We observed that IPN and TPN molecules adsorb randomly at room temperature using Scanning Tunneling Microscopy. However, these molecules undergo significant transformations upon annealing, forming chain-like structures. OPN forms disordered chains at room temperature, which become more linear and ordered upon heating. Compared to Au(111) and Ag(111), where simpler self-assemblies or dimers form, Co(0001) uniquely enables complex, ordered chain formation. This work provides critical insight into the catalytic properties of cobalt, enhancing understanding of molecular assembly on metal surfaces and offering new directions for designing nanostructured materials with precise molecular ordering.

O 22.6 Mon 18:00 P2

**Characterization of an unexpected mu3 adsorption of molecular oxygen on Ag(100) with LT-STM** — •Merve Ercelik[1], Andrés Pinar Solé[1], Liang Zhang[2], Hua Guo[2], Andreas J. Heinrich[1], Yujeong Bae[1], and Dmitriy Borodin[1] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul 03760, South Korea — [2]Department of Chemistry and Chemical Biology, Center for Computational Chemistry, University of New Mexico, Albuquerque, New Mexico 87131, USA

The interaction between molecular oxygen and metal surfaces is a key topic in quantum chemistry and surface science, with significant implications for electrochemistry and heterogenous catalysis. Using low-temperature scanning tunneling microscopy (STM), we investigate a previously unknown adsorption state of molecular oxygen on Ag(100), where the molecule binds to three silver atoms simultaneously (mu3-O2). We characterize vibrational excitations through inelastic electron tunneling spectroscopy (IETS): out-of-plane hindered rotation, in-plane hindered rotation, and in-plane hindered translation. Tunneling electron induced rotations reveal a rotational isomerization barrier of 69.3 meV. Interestingly, GGA-level DFT calculations fail to identify mu3-O2 as a stable adsorption state, likely due to self-interaction errors affecting the description of localized charges. We speculate that the mu3-O2 configuration corresponds to a formal molecular oxygen anion, with the 11 meV excitation observed in IETS attributed to a transition between spin-orbit states of the surface-bound molecular anion.

# O 23: Poster Ultrafast Electron Dynamics

Time: Monday 18:00–20:00 Location: P2

O 23.1 Mon 18:00 P2

**Charge Density Waves and Doublon Lifetime in Doped $1T$-TaS$_2$** — •J. Jayabalan[1], Gaël Reecht[1], Florian Diekmann[2], Ping Zhou[1], Walter Schnelle[3], Kai Rossnagel[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]Universität Duisburg-Essen, Germany. — [2]Christian-Albrechts-Universität zu Kiel, Germany. — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

Below a certain critical temperature, the periodic rearrangement of atoms into a long-range ordered star-like pattern transforms the metallic $1T$-TaS$_2$ into an insulating state by opening a band gap [B. Sipos, *et al.*, Nature Materials **7**, 960 (2008)]. This metal-to-insulator transition progresses through distinct charge density wave (CDW) states, driven by the interplay between electron-electron and electron-lattice interactions. In the commensurate CDW state of $1T$-TaS$_2$, the carriers excited into its upper Hubbard band (UHB), also known as a doublon state, decay in less than 20 fs due to the presence of unintentionally doped holes in the sample [M. Ligges, *et al.*, Phys. Rev. Lett., **120**, 166401 (2018)]. Through ultraviolet time-resolved photoemission spectroscopy at the Γ point, we identify a long-lived feature near the upper Hubbard band (UHB) energy in $1T$-Ta$_{(1-x)}$W$_x$S$_2$. Through variations in temperature, doping concentration, and pump-induced effects, we identify this observed feature as long-lived doublons. With STM measurements, we show a long living hole dynamics through localized excitations at specific locations of the sample. Funding by the DFG through FOR 5249 QUAST is gratefully acknowledged.

O 23.2 Mon 18:00 P2

**Ultrafast low-energy photoelectron diffraction for the study of surface-adsorbate interactions with 100 femtosecond temporal resolution** — Hermann Erk[1], Carl Erik Jensen[1], •Stephan Jauernik[1], and Michael Bauer[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

In this contribution a novel method of ultrafast electron diffraction for the study of structural dynamics at surfaces is presented. In our photoemission-based experiment we analyze the energy-momentum distribution of low-energy photoelectrons excited by a near ultraviolet (NUV) ultrafast laser pulse in graphite that are diffracted as they pass through an ordered tin-phthalocyanine adsorbate layer. The probing electron pulse is generated in the immediate vicinity of the surface. This limits the propagation distance of the electron pulse before diffraction to a few nanometers and thus minimizes pulse broadening effects due to space charge and dispersion. We experimentally demonstrate a time resolution of this ultrafast low-energy photoelectron diffraction (ULEPD) of about 100 fs [1], which is only limited by the pulse width of the NUV laser pulse and exceeds reported values of conventional ultrafast low-energy electron diffraction [2] by a factor of 10.

[1] H. Erk *et al.*, Phys. Rev. Lett. **133**, 226201 (2024)
[2] S. Vogelgesang *et al.*, Nat. Phys. **14**, 184 (2017)

O 23.3 Mon 18:00 P2

**Studying electron-phonon interaction in MoTe$_2$ using time-resolved and frequency-domain ARPES** — •Carl Eric Jensen[1], Stephan Jauernik[1], Petra Hein[1], and Michael Bauer[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

The layered transition metal dichalcogenides MoTe$_2$ and WTe$_2$ attracted significant attention in the recent years due to the topological properties of their noncentrosymmetric T$_d$-phase and their manipulation by coherent phonon excitation [1,2]. In this contribution we present time-resolved and frequency-domain ARPES (FD-ARPES) data of 1T'-MoTe$_2$. Optical excitation of the electronic system by a near-infrared (1.5 eV) pump pulse results in the excitation of coherent phonons in this material. The frequencies of the observed coherent phonon modes agree with all-optical measurements of MoTe$_2$ [2,3]. A Fouriertransform of the time-resolved ARPES data into the frequency-domain proviedes further insights into the interaction between electrons and phonons: The FD-ARPES data reveal the electronic band-selectivity of the indivitual coherent phonon modes. The results are compared with published work on WTe$_2$ [4].

[1] Sie et al. Nature 565, 61-66 (2019)
[2] Zhang et al. Phys. Rev. X 9, 021036 (2019)
[3] Fukuda et al. Appl. Phys. Lett. 116, 093103 (2020)
[4] Hein et al. Nature Communications 11, 2613 (2020)

O 23.4 Mon 18:00 P2

**Ultrafast Charge Transfer and Band Renormalization in Bilayer Graphene/single layer Ag/SiC** — •Eduard Moos[1], Zhi-Yuan 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

Intercalated monoelement metals between mono- to multi-layer graphene/SiC interfaces are a new type of van der Waals heterostructures with extraordinary properties. In the monolayer limit, silver (MLAg) exhibits a metal-semiconductor transition and enables ultrafast charge transfer between layers. Due to the twisted arrangement of the Brillouin zones, low binding energy of the valence band maximum of MLAg and the resulting band gap of bilayer graphene (BLGr), this is an interesting model system to investigate charge transfer and interlayer coupling mechanisms.

In this contribution, time- and angle-resolved photoemission spectroscopy (TRARPES) with a time resolution of 35 fs is used. The data show clear evidence for a net charge transfer between Ag and graphene on a time scale of 50 fs. On longer time scales, the electronic structure of BLGr undergoes significant changes, including an enhancement of the intrinsic splitting of the pi band as well as a reduction of the band gap. We associate these with changes in the electronic and/or structural symmetry of BLGr.

O 23.5 Mon 18:00 P2

**Ultrafast dynamics of thin films of small PAHs** — •Lorenzo Maddii Fabiani, Tobias Reiker, and Helmut Zacharias — Center for Soft Nanoscience, Busso-Peus-Str.10 48149 Münster Germany

Polycyclic aromatic hydrocarbons (PAHs), which are estimated to constitute approximately 10% of the total carbon content in space, are omnipresent in interstellar environments. Molecular reactions of molecules in space, such as ionization, fragmentation and dissociation are fundamental to the chemical evolution of the interstellar medium. To investigate the initial electronic dynamics in alternant and non-alternant PAHs in the condensed phase following optical excitation, we performed time-resolved two-photon photoemission (tr-2PPE) experiments. Thin films of PAHs were prepared on gold-coated quartz substrate. In the range from femtosecond to 200 ps up to three lifetimes after excitation of S1, S2 or S3 were observed. We provide experimental ultrafast lifetimes of nine different alternant and non-alternant small PAH molecules in thin films. For the alternant molecules an increase of the lifetimes with molecular size is found, and the lifetimes decrease generally with increasing of the probe photon energy. In contrast, non-alternant PAHs exhibited less predictable behavior. Overall, the dynamics of excited electronic states provide a fundamental basis for unraveling the reaction processes occurring within the interstellar medium.

O 23.6 Mon 18:00 P2

**Transient IR pump-probe spectroscopy on AuNP-TiO$_2$ structures** — •Lisa Mehner[1], Wouter Koopman[1], Felix Stete[1], Steven Berth[1], Alexander von Reppert[1], and Matias Bargheer[1,2] — [1]Insitute for Physics and Astronomy, University of Potsdam — [2]Helmholtz-Zentrum Berlin

Photocatalysts can enhance redox reactions by supplying energetic electrons and holes. Combining gold nanoparticles (AuNP) and TiO$_2$ nanoparticles (NP) presents a promising route for realizing broad band photocatalysts as AuNP allow broad band absorption and TiO$_2$NP provide a long excited carrier lifetime. Electrons excited in the AuNP can transfer into the semiconductor if the energy is sufficient to overcome the interfacial Schottky barrier. Transferred electrons are expected to have a prolonged lifetime in the TiO$_2$ conduction band, since no vacancies are available for recombination in the valence band. Here, we present our initial findings on charge transfer of a $TiO_2$NP+AuNP sample measured by transient pump-probe spectroscopy with optical pump-pulses and IR probe-pulses. Our measurements confirm the transfer of charges to the conduction band . Comparing $TiO_2$NP+AuNP to pure $TiO_2$NP suggests that both electron transfer from Au to $TiO_2$ as well as direct excitation of $TiO_2$ trap states occurs. The decrease in carrier lifetime with increasing fluence moreover indicates back transfer of charges from $TiO_2$ to Au.

O 23.7 Mon 18:00 P2

**Photo-induced electron pressure drives THz phonon in Platinum-Copper superlattice** — •Jan-Etienne Pudell[1], Marc Herzog[2], Max Mattern[2], Alexander von Reppert[2], Daniel Schick[3], Ulrike Boesenberg[1], Angel Rodriguez-Fernandez[1], Wonhyuk Jo[1], Roman Shayduk[1], Wei Lu[1], Felix Brause[1], Michel Hehn[5], Matias Bargheer[2,4], and Anders Madsen[1] — [1]European XFEL, Germany — [2]Institut für Physik, Uni Potsdam, Germany — [3]MBI, Berlin — [4]HZB Berlin, Germany — [5]IJL, Université Lorraine, France

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 picoseconds. This response is faster than the Debye-Waller effect, which is limited by the electron-phonon coupling time.

O 23.8 Mon 18:00 P2

**Ultrafast current response of solids - limits of quasi-classic current formula** — •Jelena Schmitz, Adrian Seith, Jan Wilhelm, and Ferdinand Evers — Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, D-93053 Regensburg, Germany

In a quasi-classical picture, the velocity of an electron with crystal momentum $\mathbf{k}$ is given by [1] $\mathbf{v}_n(\mathbf{k}) = \partial\epsilon_n(\mathbf{k})/\partial\mathbf{k} + q\,\mathbf{E}(\mathbf{t}) \times \mathbf{\Omega}_n(\mathbf{k})(1)$, where $\epsilon_n(\mathbf{k})$ denotes the band structure and $\mathbf{\Omega}_n(\mathbf{k})$ the Berry-curvature associated with the $n$-th band. Expression (1) is expected to describe the material's current response to a time-dependent external field, $E(t)$, in the limit of slow and weak driving. Motivated by recent progress in generating ultrashort laser pulses, we study the limits of applicability of Eq.(1) in the limit of fast and strong driving. To this end, we adopt the framework of the Semiconductor-Bloch Equations (SBE) [2,3]; we derive Eq.(1) using a perturbative expansion of the SBE leading to analytical expressions for the limits of applicability and compare Eq.(1) with numerical solutions of the full SBE [4].

For massive Dirac Fermions, we find the bandgap energy and the Fermi level as the parameters determining the frequency domain as well as the maximum $E$-field strength for which the SBEs lead to matching results with Eq.(1).We also calculate corrections to Eq.(1) that enable us to identify Berry-curvature terms at higher frequencies.[1] Xiao, Di et. al., Rev. Mod. Phys. 82, 1959 (2010) [2] Schmitt-Rink, Stefan et. al., Phys. Rev. B 37, 941 (1988) [3] Wilhelm, Jan et. al., Phys. Rev. B 103, 125419 (2021) [4] https://github.com/ccmt-regensburg/CUED/

O 23.9 Mon 18:00 P2

**XUV pulses with variable photon energy, pulse duration and bandwidth for time-resolved ARPES** — •Isabella Alexandra Hofmeister, Niklas Hofman, Michael Schildbach, and Isabella Gierz — University of Regensburg, Regensburg, Germany

Time- and angle-resolved photoemission spectroscopy (trARPES) provides an unprecedented view on non-equilibrium quasiparticle dynamics and band structures in momentum space. Extreme ultraviolet (XUV) pulses generated by high harmonics generation (HHG) in noble gases are usually required to gain access to the complete first Brillouin zone. HHG yields a broad spectrum containing all the odd harmonics of the driving frequency up to a cut-off energy determined by the intensity and frequency of the drive. Therefore, a single harmonic is typically selected for trARPES using grating monochromators, multilayer mirrors, or a combination of filters. We compare different approaches implemented in a single trARPES setup with respect to their bandwidth and pulse duration and present strategies to enable complementary trARPES measurements with either good energy or good temporal resolution.

O 23.10 Mon 18:00 P2

**Terahertz Excitation Source for Next Generation Time-of-Flight Momentum Microscopy at FLASH** — Michael Herb[1], •Stefan Miedaner[1], Thomas Seitz[1], Jure Demsar[2], Stephan Winnerl[3], and Isabella Gierz[1] — [1]University of Regensburg, Germany — [2]Johannes Gutenberg University of Mainz, Germany — [3]Helmholtz Center Dresden-Rossendorf, Germany

We will combine the broad spectral tunability of the free-electron laser FLASH with Terahertz excitation for next-generation time-of-flight momentum microscopy (ToF-MM). This unique combination will enable unprecedented access to the non-equilibrium electronic and structural properties of novel quantum materials using a variety of time-resolved spectroscopic, diffraction, and microscopic techniques. This requires the design and installation of a compact Terahertz pump source operating at Megahertz repetition rate. Here, we present the current status of the photoconductive-emitter-based source [1] and its characterization by electro-optic sampling.

[1] Optics Express 29, 427247 (2021)

O 23.11 Mon 18:00 P2

**table-top source for x-ray absorption spectroscopy with photon energies upto 350 eV** — •Rajdwip Bhar, Oscar A. Naranjo-Montoya, Lukas Kalkhoff, Marika Schleberger, Heiko Wende, Alexander Tarasevitch, and Uwe Bovensiepen — University of Duisburg-Essen, Duisburg, Germany

Material science research aims to understand electronic properties and dynamics of complex materials. Performing pump-probe experiments using optical pump and x-ray probe enables capturing element-specific snapshots of the pump induced changes in a material. This contribution describes the development of a tabletop soft x-ray spectroscopy setup based on high harmonic generation using noble gases in a hollow core waveguide (HCW) [1].

To generate high harmonics with higher photon energies, a near-infrared driving laser source based on optical parametric chirped-pulse amplification (OPCPA) was developed [2]. Starting with an 800 $nm$ seed and a 1030 $nm$ pump, the OPCPA generates 1.5 $\mu m$ and 3 $\mu m$ pump pulses with pulse energies of 1.8 $mJ$ and 0.8 $mJ$, respectively. The 1.5 $\mu m$ pulses, compressed to $\sim$ 40 $fs$ using chirped mirrors, pump the HCW, generating harmonics that reach photon energies up to 350 $eV$. Near-edge x-ray absorption spectroscopy at the B $K$-edge in crystalline boron and hexagonal boron nitride (hBN) samples was performed, showing excellent agreement with literature data.

[1] O. A. Naranjo-Montoya et al., Review of Scientific Instruments **95**, 103001 (2024).

[2] M. Bridger et al., Opt. Express **27**, 31330-31337 (2019).

O 23.12 Mon 18:00 P2

**New end-station for time- and angle-resolved photoelectron spectroscopy in Artemis facility** — •Yu Zhang, Charlotte E. Sanders, Bruce Weaver, Tiffany Walmsley, James O. F. Thompson, Richard T. Chapman, and Emma Springate — Central Laser Facility, STFC Rutherford Appleton Laboratory, Research Complex at Harwell, Harwell, United Kingdom

Artemis, located at the Central Laser Facility in the UK, is a user facility offering time- and angle-resolved photoelectron spectroscopy (TrARPES) utilizing extreme ultraviolet (20-45 eV) photon sources based on high harmonic generation of ultrafast laser. After more than a decade of operation, Artemis has established itself as a leading facility in the research of ultrafast electron dynamics on surfaces. Recently, Artemis received an significant upgrade of its end-station, which will provide users with state-of-the-art techniques in ultrafast time-resolved measurements. These new capabilities include both momentum and real-space mapping, large-angle E-k mapping with a deflector, and a closed-loop cryostat for low-temperature measurements. Detailed information about these features can be found in the poster. Along with the recently upgraded 100kHz laser source, Artemis is committed to delivering high-performance TrARPES for its user communities.

O 23.13 Mon 18:00 P2

**Temporal evolution of surface plasmon polariton skyrmions** — •Philipp Gessler, Alexander Neuhaus, Maria Azhar, Pascal Dreher, Frank Meyer zu Heringdorf, and Karin Everschor-Sitte — University of Duisburg-Essen, Germany

In recent years, structures reminiscent of those found in magnets [1] have been predicted and observed in Surface Plasmon Polaritons (SPPs). Of particular interest are topological SPP structures such

as skyrmion lattices [2,3] or merons [4]. In particular, these structures have been identified in various quantities related to the electric field, many of which exhibit amplitudes that oscillate over time. Building on insights from micromagnetism, our objective is to explore the dynamic behavior of these novel SPP states beyond mere temporal oscillations.
[1] C. Back et al., J. Phys. D: Appl. Phys. **53**, 36 (2020)
[2] S. Tsesses et al., Science **361**, 6406 (2018)
[3] T. J. Davis et al., Science **368**, 6489 (2020)
[4] Y. Zheng et al., Nanophotonics **13**, 2 (2024)

O 23.14 Mon 18:00 P2

**Femtosecond momentum microscopy of field-effect gated bilayer $WSe_2$ and monolayer graphene** — •Bent van Wingerden, Jan Philipp Bange, Jonas Pöhls, Wiebke Bennecke, Paul Werner, Daniel Steil, Matthijs Jansen, R. Thomas Weitz, Marcel Reutzel, and Stefan Mathias — I. Physikalisches Institut, Georg-August Universität Göttingen, Germany

Atomically-thin transition metal dichalcogenides and their respective Moiré heterostructures can host a variety of strongly correlated electronic phases, such as Wigner crystals and Mott insulators. The formation of these phases critically depends on the precise occupation of the corresponding Moiré superlattice states [Regan *et al.* Nature 579, (2020)], and might therefore be controlled by field-effect doping of charge carriers [Nguyen *et al.* Nature 572 (2019)]. In our work, we realized this in combination with a table-top time-resolved ARPES setup, i.e. our Göttingen femtosecond momentum microscopy experiment [Schmitt *et al.*, Nature 608, (2022)]. Our extension of ARPES experiments on field-effect gated heterostructures into the time domain on a laboratory scale will facilitate the study of non-equilibrium dynamics of strongly correlated phases and charged quasiparticles, e.g. trions. We provide proof-of-principle data on field-effect gated monolayer graphene and present time-resolved photoemission data of a $WSe_2$ bilayer at different charge carrier densities.

O 23.15 Mon 18:00 P2

**Towards ultrafast momentum microscopy of exciton dynamics at ZnO surfaces** — •Hashima Marukara, Junde Liu, and Stefan Mathias — Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany

The semiconductor ZnO, known for its wide band gap and high exciton binding energy, stands out as a promising material among transparent conductive oxides for applications in optoelectronics and catalysis[1,2]. Surface excitons, i.e. bound electron-hole pairs localized at the material's surface, play a crucial role in mediating its optical and electronic properties, significantly influencing energy conversion processes at the surfaces [3]. An ideal tool to study these ultrafast processes is time- and angle-resolved photoelectron spectroscopy, which gives access to the exciton landscape and the relevant excitation and relaxation pathways. In our new project within the CRC1633 "Proton-coupled electron transfer", we aim to study the ultrafast surface exciton dynamics at the ZnO(10-10) surface using our Göttingen time-resolved momentum microscopy setup. By using this technique, which gives us access to full energy and momentum space, we aim to gain detailed information on the ZnO's exciton momentum and real-space properties (localized/delocalized/defect/etc.) and the accompanying exciton dynamics [4].

[1] Gierster et al., Nat Commun 12, 978 (2021)
[2] Foglia et al., Struct. Dyn. 6, 034501 (2019)
[3] Deinert et al., Phys. Rev. Lett. 113 057602 (2014)
[4] Reutzel et al., Advances in Physics X 9, 2378722 (2024)

O 23.16 Mon 18:00 P2

**Towards momentum microscopy of plasmon excited $WSe_2$** — •Mattis Langendorf[1], Paul Werner[1], Marco Merboldt[1], Jan Philipp Bange[1], Wiebke Bennecke[1], Jonas Pöhls[1], Tobias Meyer[2], Thomas R. Weitz[1], Marcel Reutzel[1], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany — [2]Georg-August-Universität Göttingen, Institut für Materialphysik, Germany

Femtosecond momentum microscopy represents a uni measurement technique that effectively integrates the advantages of angle-resolved photoemission spectroscopy (ARPES) and photoelectron emission microscopy (PEEM) within a single microscope. The capacity to transition between real- and momentum-space imaging in time-resolved photoelectron spectroscopy enables the investigation of quasiparticles in both regimes [Bange et al., Nature Photonics, in press (2024)]. In this contribution, we pursue the characterization of electron-hole pairs, i.e. excitons, which were excited by a collective excitation of charge carriers, i.e. a surface plasmon polariton (SPP). In this approach, the propagating SPPs are imaged with photoemission electron microscopy, and the formation of excitons in the TMD is then visualized with time-resolved dark-field imaging techniques.

O 23.17 Mon 18:00 P2

**Control and manipulation of low-energy electrons** — •Dennis Epp[1], Frank Long[1,2], Benjamin Schröder[1], and Claus Ropers[1,2] — [1]Max-Planck-Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

In surface science and materials physics, electron pulses are a powerful probe of structural dynamics in time-resolved diffraction and microscopy experiments. A fundamental challenge lies in the Coulomb interaction [1] and initial energy distribution, which negatively affects the electron beam size and pulse duration after propagation towards the sample. Active control of electron pulse properties by compression schemes has proven to enhance temporal resolution [2-4]. This is particularly important for low-energy electrons and their high dispersion due to low propagation velocity [4]. In this paper, we demonstrate longitudinal and transversal phase-space manipulation of low-energy electron pulses using synchronized RF fields in the gigahertz frequency range [4]. Furthermore, novel beam shaping concepts including electron pulse streaking, compression and deflection are discussed.

[1] van Oudheusden, et al., Physical Review Letter 105, 264801 (2010). [2] Kassier, et al., Applied Physics B 109, 249-257 (2012). [3] Epp, et al., Structural Dynamics 11, 024306 (2024). [4] Haindl, et al., Nature Physics 19, 1410*1417 (2023).

O 23.18 Mon 18:00 P2

**Band-resolved studies of laser-induced ultrafast dynamics in gold** — •Stephanie Roden, Tobias Held, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU in Kaiserslautern

The irradiation of a metal with a short-pulsed optical laser leads to the excitation of electrons, which absorb energy in accordance with their orbital characteristics. To analyze the resulting state of thermodynamic non-equilibrium, the thermalization of the excited electrons and relaxation processes with the phonon system to a joint temperature can be calculated in a kinetic manner by coupled Boltzmann collision integrals.

In this work we extend our existing energy-resolved model based on one effective band for the electrons [1] to a two-band model for a thin metal film that distinguishes between the free sp- and more localized d-electrons [2]. By considering the different electron bands separately, we can investigate the influence of intra- and interband relaxation in the electron system on the dynamics of the entire sample. We are focusing especially on the effect on the band occupation and the coupling strengths between the electron systems and the phonons.

[1] B. Y. Mueller and B. Rethfeld, PRB 87, 035139 (2013)

[2] T. Held, S. T. Weber, and B. Rethfeld, Journal of Physics: Condensed Matter (2025)

O 23.19 Mon 18:00 P2

**Ultrafast intra- and interlayer charge transfer at the FePc/$WSe_2$ interface** — •Gregor Zinke[1], Sebastian Hedwig[1], Benito Arnoldi[1], Martin Anstett[1], Lu Lyu[1,2], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern - Landau, Erwin-Schroedinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Experimental Physics II, Institute for Physics, University of Augsburg, Universitätsstraße 1, 86159 Augsburg

Tailoring the optoelectronic properties of 2D-van-der-Waals materials by material design is a promising approach for functionalizing charge and spin carriers in low-dimensional materials. In this work, we demonstrate how optically excited ultrafast charge carrier dynamics of TMDCs can be altered by the formation of molecule/2D material heterostructures. Here, we focus on an ordered FePc monolayer film deposited on the surface of a bulk $WSe_2$ crystal. Using time- and angle-resolved photoemission in a VIS-pump, XUV-probe setup, we will elucidate the ultrafast response of the electronic system to an optical excitation on fs-timescales. Of particular interest is the investigation of intra- and interlayer charge carrier dynamics at the FePc / $WSe_2$ interface, which can be disentangled by the characteristic momentum space signatures of the $WSe_2$ Bloch-like states and molecular orbitals. We will further illustrate the impact of ultrafast charge separation across the interface on transient changes of the interfacial energy level alignment.

O 23.20 Mon 18:00 P2

**Influence of ballistic electrons on temperature equilibration in bulk gold** — •Lukas Jonda, Tobias Held, Markus Uehlein, Christopher Seibel, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics andResearch Center OPTIMAS, RPTU Kaiserslautern-Landau

During femtosecond laser irradiation of gold, electrons are excited to a state of non-equilibrium in space and energy. Highly excited electrons transport energy ballistically into the bulk due to their relatively long mean free path. On a picosecond timescale, electrons transfer energy to the crystal lattice via electron-phonon collisions.

The objective of this study is to analyze the influence of non-equilibrium electrons on energy transport. Therefore, a two-temperature model will be coupled with a kinetic Monte Carlo simulation. With the former we describe diffusive transport as well as the electron-phonon equilibration, while the latter describes the primary electron excitation by the laser pulse, secondary electron generation, and transport of non-equilibrium electrons above the Fermi level.

O 23.21 Mon 18:00 P2

**Hot carrier dynamics and band gap formation in lead intercalated graphene on Ni(111)** — Martin Mitkov[1], Lu Lyu[2], Eva Walther[1], Martin Anstett[1], •Alexander Schmid[2], Christina Schott[1], Gyula Halasi[3], Nikolett Oláh[3], Csaba Vass[3], Zoltán Filus[3], László Óvári[3], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]RPTU Kaiserslautern-Landau — [2]University of Augsburg — [3]ELI ALPS, Szeged, Hungary

The intercalation of atoms between 2D materials and surfaces offers an intriguing opportunity to tune spin functionalities at surfaces. The combination of heavy metal atoms and magnetic surfaces allows to tune the band structure of 2D materials through the interplay of spin-orbit coupling and magnetic proximity effects. In this poster, we present our recent findings on the band structure and hot electron dynamics of a Pb-intercalated graphene layer on Ni(111).

The highly reactive Ni substrate causes a charge transfer into the graphene layer, which leads to n-doped Dirac cones. Pb intercalation leads to a decoupling of the graphene, resulting in a quasi-free standing graphene layer on Ni.

Our time-resolved momentum microscopy experiment allows us to determine the influence of Pb intercalation on the ultrafast carrier dynamics of the Gr/Ni(111) interface. We discuss the momentum space distribution of the optically excited carriers at the K-point for the bare and Pb intercalated graphene and present indications for a modification of the magnetization dynamics of the Ni substrate by energy and charge transfer from the Pb-intercalated graphene.

## O 24: Poster Scanning Probe Techniques: Method Development

Time: Monday 18:00–20:00 Location: P2

O 24.1 Mon 18:00 P2

**Comparative Analysis of Work Function Measurements Using STM/AFM Techniques** — •Daryoush Nosraty Alamdary, Matthias Bode, and Artem Odobesko — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The engineering of the work functions at the interface of complex materials is sometimes the key [1] for an energy band tuning that supports proximity-induced effects [2]. While there are handful of established methods that allow a precise measurement and determination of the work function, STM-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 3 different techniques based on a combined STM/AFM setup. For a few well-characterized sample systems we analyze the benefits and difficulties of each method. Finally, we draw a conclusion as to which method is the more precise and reliable method, whereby the special focus lies on the accuracy and the challenges of the interpretation.

[1] P. Rüßmann em et al., Proximity induced superconductivity in a topological insulator, arXiv:2208.14289 (2022)

[2] L. Fu and C. L. Kane, Superconducting Proximity Effect and Majorana Fermions at the Surface of a Topological Insulator, Phys. Rev. Lett. **100**, 096407 (2008)

O 24.2 Mon 18:00 P2

**Cryogenic, ultrahigh vacuum sample transfer between electrospray ion beam deposition (ESIBD) and scanning probe microscopy (SPM)** — •Alejandro Lynch Gonzalez, Stephan Rauschenbach, Lukas Eriksson, Benjamin Mallada, Tim Esser, and Marko Grabarics — University of Oxford

Electrospray ion beam deposition (ES-IBD) is currently the only viable method for cleanly and selectively depositing large and complex molecules which do not have a vapour pressure while preserving their chemical structure. In our lab, ESIBD[1] and SPM instruments are physically separate and sample transfer between them is performed using a vacuum suitcase system which maintains UHV and cryogenic conditions during transfer, essential for suppressing surface diffusion, conformational changes, and contamination during the transfer. Here, we present the design, implementation, and benchmarking of a cryogenic UHV suitcase and showcase applications.

[1] Fremdling, P. et al. ACS nano 16, 14443-14455 (2022).

O 24.3 Mon 18:00 P2

**Ultra-broadband Terahertz Time-Domain Spectroscopy for Space Exploration** — •Dominic Azih[1,2], Yookyung Ha[2], Jonas Woeste[1,2], Nikola Stojanovic[2], and Michael Gensch[1,2] — [1]Technical University, Berlin, Germany — [2]DLR Ínstitute of Optical Sensor Systems, Berlin, Germany

Femtosecond lasers have in recent years been shown to be space qualified and with the development of compact femtosecond laser systems [1,2], Terahertz Time-Domain Spectroscopy (THz TDS) allows meanwhile to cover an essential part of the molecular fingerprint spectral range and has several technological advantages over the commonly used Fourier-Transform Infrared techniques (FTIR). The advantages are compactness, replacement of components (cryogenic) spectrally broadband infrared detectors with electro-optic/acousto-optic photonic techniques and the potential to be chip-integrable. Here we show our progress enroute to a THz time-domain spectroscopic setup for space applications with a bandwidth of over 30THz and a resolution of better than 100GHz [3].

O 24.4 Mon 18:00 P2

**High-collection efficiency optical scanning probe microscopy with on-axis parabolic mirror** — •Aleksander Bogucki[1], Magdalena Grzeszczyk[1], Yeon-ji Kim[1], Yewon Kim[1], German Orlov[1], Lei Fang[1], Wonjun Jang[1,2], and Andreas Heinrich[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul, South Korea — [2]Department of Physics, EWHA Womans University, Seoul, South Korea

Scanning probe microscopy (SPM) techniques are essential for investigating surface physics, from single atoms to complex systems like organic molecules. Combining SPM with optical spectroscopy enhances our ability to explore system dynamics. However, existing setups face photon collection efficiency challenges due to spatial constraints, particularly for systems with long-lived excited states.

We present a homemade optics-integrated scanning probe microscope using a centered on-axis parabolic mirror with a short focal length. The scanning component employs a combined AFM/STM qPlus sensor with a long tip. Free-beam optics maximize photon collection efficiency, reaching an estimated upper limit of 90%. This design eliminates chromatic aberrations, enables polarization measurements, and operates under ultra-high vacuum (UHV) at low temperatures (4K), ensuring high stability and precision.

O 24.5 Mon 18:00 P2

**Electron wavefront shaping with light** — •martino zanetti[1,2], Tilman Kraeft[1,2], Luis Alfredo Ixquiac Mendez[1,2], Alexandra Pernishova[1,2], and Thomas Juffmann[1,2] — [1]University of Vienna, Faculty of Physics — [2]University of Vienna, Max Perutz Laboratories

Electron Microscopes (EM) are common and fundamental tools in many research fields, as they can image samples with resolutions down to the nanometric scale. The ability to arbitrarily shape the electron beam of an EM with light can help overcome intrinsic limits like electron lens aberrations and pave the way to new EM techniques [1].

For shaping the electron beam, a modified Scanning-EM is coupled to a high-power pulsed laser. The electron-light interaction takes place in the SEM chamber. The electrons are then detected after free propagation to measure their spatial distribution. Here, we present our advancements in applying the electron beam shaping technique to demonstrate single electron wavefront modulation. The intensity profile of a TEM01 laser mode is imprinted on the wavefront of the electron, which thus resembles that of an electron going through a double slit. Adding up the detection of multiple electrons, we expect to see an interference pattern that proves the effective modulation of the electron wavefront. The need for micrometric resolution measurements required us to develop a single-electron detector which outperforms many commercially available ones in the 20-30 keV range, being at the same time more flexible and cheaper.

[1] Mihaila et al., Phys. Rev. X 12, 031043 (2022)

O 24.6 Mon 18:00 P2

**Optimizing ESR-STM for mK Temperatures in a Closed-Cycle Dilution Refrigerator** — •Luise Renz, Máté Stark, Jonas Arnold, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Using Electron Spin Resonance (ESR) combined with Scanning Tunneling Microscopy (STM), electronic and magnetic properties of single atoms and molecules can be studied. However, the possibility of applying RF voltages to the tip often limits the achievable minimum temperature of the STM. We here describe an ESR-STM setup mounted in ultra-high vacuum (UHV) in a closed-cycle Dilution Refrigerator (DR). The focus here is on the wiring of the STM, the material choice and the filtering of the RF and DC cables with the goal of having a good transmission of the RF lines but nevertheless also mK-temperatures in the STM junction. The resulting bandwidth and transmission of these cables, the noise level of the STM as well as the electronic temperature of the STM junction, is presented. The electronic temperature is estimated on a Pb(111) crystal by evaluating the superconducting gap and the Josephson peak (using a superconducting tip).

O 24.7 Mon 18:00 P2

**Detection and Localization of Atoms and Molecules on Different Surfaces Using Computer Vision** — •Lovis Hardeweg, Johannes Schwenk, Wantong Huang, Kwan-Ho Au-Yeung, Máté Stark, Paul Greule, Christoph Sügers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Scanning Probe Microscopy (SPM) methods are unparalleled in their ability to image and manipulate structures on the atomic scale. In combination with machine learning techniques, this allowed to automate processes such as removing a molecule from a thin layer [1] or moving an adsorbed molecule to a specific position [2]. However, this often relies on prior human interaction to identify and localize objects of interest, like a thin film or a single adsorbate. Here, we discuss methods that automate several steps in SPM experiments, with the goal of advancing single atomic and molecular spin detection experiments. For that, we employ computer vision techniques to STM topography data and are able to extract information, such as the location of single atoms and molecules or the presence of different sample surfaces, for instance ultra-thin MgO films grown on Ag(001). We believe that these abilities, once sufficiently developed, can lead to a significant reduction in the need for human intervention in the automated use of high-resolution low temperature SPM. [1] P. Leinen et al. Sci. Adv., vol. 6, no. 36, p. eabb6987, Sep. 2020, doi: 10.1126/sciadv.abb6987. [2] B. Ramsauer et al. J. Phys. Chem. A, vol. 127, no. 8, pp. 2041-2050, Mar. 2023, doi: 10.1021/acs.jpca.2c08696.

O 24.8 Mon 18:00 P2

**A Closed-Cycle Atomic Force Microscopy Setup for Electron Spin Resonance Measurements at mK Temperatures** — •Adrian Seiler, Lovis Hardeweg, Luise Renz, Arian Vosoghi Marand, Kwan Ho Au-Yeung, Wantong Huang, Paul Greule, Máté Stark, Christoph Sürgers, Wolfgang Wernsdorfer, Johannes Schwenk, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Combining scanning probe techniques with electron spin resonance (ESR) provides a unique tool for the investigation as well as the manipulation of individual surface-adsorbed spins. Most experiments up to date are relying on Scanning Tunneling microscopy (STM) and thus conductive samples [1]. As a result, scattering of electrons with the spin system is a major source of decoherence and relaxation. In contrast, atomic force microscopy (AFM) provides the possibility to reduce the scattering intensity with the conducting electrodes. Here, we present the first implementation steps of a commercial AFM head and ultra-high vacuum setup in a compact dilution refrigerator. The final setup is designed to reach milli-Kelvin temperatures ($\approx 50$ mK) with short cool-down times on the order of several hours. In addition to the dilution unit, the system utilizes a closed-cycle cryocooler allowing longtime stable operation. We further improve the time-consuming sample preparation by automation of the sputter and annealing process to allow for a rapid turnaround of samples in the future.

[1] Y. Chen et al. Adv. Mater. 35, 2107534 (2023).

O 24.9 Mon 18:00 P2

**Lightwave driven magnetic field scanning tunneling microscopy** — •Leo Ringer, Andreas Rank, Peter Menden, Christian Meineke, Rupert Huber, and Jascha Repp — University of Regensburg, Regensburg, Germany

Lightwave driven scanning tunneling microscopy (LW-STM) is based on the key idea to directly steer electron tunneling in STM by ultrashort light pulses. Combining the development of LW-STM with a tunable magnetic field would allow following spin dynamics - e.g. spin precession - in molecules and other atomistic structures with single-electron sensitivity. To this end, we develop a novel lightwave driven scanning tunneling microscope including an external magnetic field to resolve single-spin dynamics with atomic spatial and ultrafast temporal resolution. Instrumental challenges of this development will be discussed, and we present the resulting instrument design including the head of the scanning tunneling microscope, the laser source as well as the solution to introduce the laser transient from outside the vacuum system to the tip-sample junction.

O 24.10 Mon 18:00 P2

**Implementation of radio-frequency magnetic fields for electron spin resonance atomic force microscopy** — •Raffael Spachtholz, Lisanne Sellies, Franziska Bruckmann, Sonja Bleher, Philipp Scheuerer, and Jascha Repp — Department of Physics, Universität Regensburg

Implementing electron spin resonance in scanning tunneling microscopy represents a milestone in controlling spin systems at atomic scales [1]. In this emerging research field the required radio-frequency (RF) signal is provided as an electric field, translating to an effective magnetic field.

Here we report the integration of a radio-frequency (RF) magnetic field, in the frequency range of 0.1 to 3 GHz, into a scanning-probe microscope. We utilized a flexible polyimide printed-circuit-board coil to generate the RF magnetic fields. Additionally, an insulating sample, coated with a gold microstructure, was designed to locally enhance the RF magnetic field while mitigating the screening effects caused by a metallic substrate. Up to 3 GHz the transmission only moderately depends on frequency and exhibits no sharp resonances. This development enabled the implementation of electron spin resonance in atomic force microscopy, as demonstrated for individual pentacene molecules [2].

[1] S. Baumann, et al., Science 350, 417-420 (2015)

[2] L. Sellies, et al., Nature 624, 64-68 (2023)

O 24.11 Mon 18:00 P2

**Implementation and characterization of all-electronic pump-probe spectroscopy on a low-temperature scanning tunneling microscope** — •Guido Hiller, Gaël Reecht, and Manuel Gruber — Universität Duisburg Essen, Duisburg

Pump-probe spectroscopy is a powerful technique for investigating non-equilibrium dynamics, where the time resolution is determined by the duration of the pump and probe pulses rather than the detectors bandwidth. When combined with a scanning tunneling microscope (STM), this method enables dynamic measurements at the level of individual atoms and molecules, achieving both high temporal and spatial resolutions [1].

In this work, we implement an all-electric pump-probe scheme on a low-temperature STM. Cross-correlation measurements on an Au(111) surface reveal a time resolution of 100 ns. This resolution is constrained by the broadening of voltage pulses during transmission to the STM junction [2]. To address this, we conducted a detailed analysis of the frequency-dependent transmission function of the instrument. Funding support from the CRC 1242 is gratefully acknowledged.

[1] Loth et al., Science 329, 1628 (2010)

[2] Herve et al., Applied Physics Letter 107, 093101 (2015)

## O 25: Overview Talk Jörg Kröger

Time: Tuesday 9:30–10:15 Location: H24

**Topical Talk** O 25.1 Tue 9:30 H24

**Exploring quantum physics with scanning probe methods** — •Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, Germany

It is hardly possible to ignore the importance of scanning probe techniques for the understanding of mechanisms and principles in the quantum behavior of condensed matter. This Overview Talk presents contributions of atomic force microscope experiments to controlling and quantifying interactions involved in bonding processes at the single-atom level. It then demonstrates that scanning tunneling spectroscopy is successfully used in exciting and detecting quantum vibrations and spins as well as in characterizing the charge transport across the metal-superconductor interface. Funding by the DFG through KR 2912/17-1, 18-1, 21-1 and the BMBF through ForLab is acknowledged.

## O 26: Focus Session Ultrafast Electron Microscopy at the Space-Time Limit III

Shaping functionalities on the nanoscale is one of the most essential challenges in modern condensed matter research. It requires a comprehensive understanding of the complex interplay of the electronic, spin, and lattice degrees of freedom in materials and requires tailoring energy transfer and dissipation pathways on the smallest length and fastest timescales. Recent instrumentation breakthroughs in different varieties of pump-probe ultrafast electron microscopy have opened the way for accessing electronic and structural dynamics at surfaces, interfaces, and nanostructures with down-to-attosecond resolution in time. While ultrafast photoemission electron microscopy techniques provide supreme sensitivity to spin and electron dynamics in real momentum space, bright ultrashort electron pulses in the ultrafast implementation of more traditional electron microscopes can probe optical states, local magnetization, and lattice dynamics with a nanometer spatial resolution.

This focus session highlights recent advances in ultrafast high-resolution electron probing. These include new instrumentation and techniques, excitations from the THz to X-ray regime, and studying novel phenomena and materials systems. At the same time, it will bring together researchers from the different areas of ultrafast condensed matter physics to foster discussions and new collaborations to explore emergent scientific questions in this field.

Organized by
Armin Feist (MPI Göttingen) and Benjamin Stadtmüller (University Augsburg).

Time: Tuesday 10:30–13:00 Location: H2

**Invited Talk** O 26.1 Tue 10:30 H2

**Attosecond Electron Microscopy** — •Peter Baum — Universität Konstanz, Germany

All processes in materials, nanostructures and devices are on a fundamental level defined by electronic and atomic motion from initial to final conformations. Our approach for a direct, real-space visualization is pump-probe electron diffraction and microscopy with single-electron wavepackets under the control of laser light. The resulting few-femtosecond and attosecond time resolution allows to see almost any light-matter interaction or structural dynamics on fundamental scales in space and time. We report selected results on strongly correlated materials, rotational phonons, electronic circuitry, free-electron quantum phenomena and attosecond dynamics in nanomaterials.

O 26.2 Tue 11:00 H2

**Steady-State and Time-Resolved Cathodoluminescence of III-Nitride Semiconductors** — •Kagiso Loeto, Aidan Flynn Campbell, Domenik Spallelk, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Deutschland

Cathodoluminescence (CL), in steady-state and time-resolved modes, has advanced the study of semiconductor optical properties, crucial for microelectronics and III-nitride optoelectronics. A new state-of-the-art time-resolved CL (TRCL) microscope at the Paul-Drude-Institut features a high-performance SEM with a stable electron source and advanced light collection system, enabling optimized imaging and high spatial resolution at acceleration voltages as low as 0.35 kV. The system features a UV-optimized CCD camera for studying UV-emitting materials like III-nitrides. Time-resolved operation is enabled by an ultrafast beam blanker paired with detectors achieving temporal resolutions of tens of picoseconds, offering new insights into the dynamic optical properties of advanced semiconductors. It will be employed in three focus areas, highlighting its distinct capabilities. First, very-low acceleration voltage operation will enable high-resolution mapping of individual point defects in AlGaN quantum well structures, revealing their impact on AlGaN-based UV LEDs. Second, ultraviolet-optimized photon detectors will study temperature-stable excitonic bands in AlN with high spectral resolution, providing insights into their origins. Lastly, the instrument's time-resolved capabilities combined with spatial mapping will explore the interplay between carrier dynamics and localization in InGaN pseudosubstrates.

O 26.3 Tue 11:15 H2

**Spin Resonance Spectroscopy meets Transmission Electron Microscopy** — •Philipp Haslinger — Atominstitut, USTEM, Technische Universität Wien, Austria

Coherent spin resonance methods such as nuclear magnetic resonance and electron spin resonance spectroscopy have led to spectrally highly sensitive, non-invasive quantum imaging techniques. Here, we will present a spin resonance spectroscopy approach developed for transmission electron microscopy [1,2] and will explain different techniques to sense with electrons for microwave manipulated spin states of the sample. This could enable state-selective observation of spin dynamics on the nanoscale and indirect measurement of the environment of the spin systems, providing information on, for example, atomic structure, local chemical composition and neighbouring spins.

[1] P. Haslinger, S. Nimmrichter, and D. Rätzel, Spin Resonance Spectroscopy with an Electron Microscope, Quantum Sci. Technol. 9, 035051 (2024). [2] A. Jaroš, J. Toyfl, A. Pupić, B. Czasch, G. Boero, I. C. Bicket, and P. Haslinger, Electron Spin Resonance Spectroscopy

in a Transmission Electron Microscope, arXiv:2408.16492 (2024).

O 26.4 Tue 11:30 H2

**Observation of Kapitza-Dirac effect with fast electrons** — •Kamila Moriová[1], Petr Koutenský[1], Marius Constantin Chirita Mihaila[1], Zbyněk Šobáň[2], Andreas Schertel[3], Jaromír Kopeček[2], and Martin Kozák[1] — [1]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [3]Carl Zeiss AG, Oberkochen, Germany

Advancing ultrafast electron microscopy relies on coherent control of free electron wavefunctions. While most research focuses on electron interactions with optical near-fields, an all-optical approach using ponderomotive forces offers a promising alternative for manipulating pulsed electron beams. The Kapitza-Dirac effect [1], where free electrons diffract coherently from a standing light wave, enables momentum transfer via stimulated Compton scattering. However, its application has been limited to low-energy electrons due to challenges in resolving small deflection angles of electron beams caused by photon absorption and emission.

We report the observation of the Kapitza-Dirac effect in a scanning electron microscope using high-energy (20 keV) electrons. Photon sidebands in the electron transverse momentum spectrum are detected in a convergent beam diffraction geometry using spatial filtering. This effect can serve as a coherent electron beam splitter or phase plate in various types of electron microscopes and paves the way for exploring fundamental electron-light interactions.

[1] Freimund, D. L. et al. Nature 413, 142 (2001)

O 26.5 Tue 11:45 H2

**Recent results of the ultrafast scanning electron microscope in Erlangen** — •Stefanie Kraus[1], Tomas Chlouba[1], Roy Shiloh[1], Leon Brückner[1], Julian Litzel[1], Zhexin Zhao[1], Viacheslav Korolev[1], Manuel Konrad[1], Tatsunori Shibuya[1,3], and Peter Hommelhoff[1,2] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — [2]Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München — [3]AIST, Tsukuba, Japan

Ultrafast electron microscopy is revolutionizing the capabilities of electron microscopes, allowing for unprecedented spatial and temporal resolution. Closely related is the coupling of electrons and optical nearfields, which is based on the excellent electron pulse properties an ultrafast scanning electron microscope (USEM) can provide. We have leveraged the interaction of electrons with the near field of a periodic structure to achieve sub-femtosecond electron pulse compression as well as laser acceleration of electrons. This advancement enhances temporal resolution and facilitates large beam energy variations, enabling detailed investigations of ultrafast dynamics. In this talk, we will provide an overview of our recent progress, including electron energy modulation in larger structures illuminated with 10 micrometer light as to enhance the current throughput, electron bunch compression, and the latest experimental results.

O 26.6 Tue 12:00 H2

**FEL-based core-cum-conduction momentum microscopy of ultrafast charge-density-wave dynamics** — •N. Wind[1,2,3], M. Heber[1,3], D. Kutnyakhov[1], L. Wenthaus[1], J. Dilling[2], L. Bruckmeier[2], S. Chernov[1], O. Tkach[4], A. Mehta[5], J. Koralek[5], G. Dakovski[5], J.A. Sobota[6], P.E. Majchrzak[6], D. Puntel[6], D. Liu[6], G. Schönhense[4], H.J. Elmers[4], Z.X. Shen[6], M. Scholz[1], and K. Rossnagel[1,2] — [1]Deutsches Elektronen Synchrotron DESY, 22607 Hamburg, Germany — [2]Christian-Albrechts-Universität zu Kiel IEAP, 24098 Kiel, Germany — [3]Universität Hamburg, IExP, 22761 Hamburg, Germany — [4]Johannes Gutenberg-Universität, Institut für Physik, 55128 Mainz, Germany — [5]SLAC National Accelerator Laboratory, Menlo Park, CA 94205, USA — [6]Stanford University, Institute for Materials and Energy Science, CA 94305, USA

Transition-metal dichalcogenides (TMDCs) offer a rich platform for studying novel forms of quantum and nanoelectronics in layered structures approaching the 2D limit. Among them, 1-$T$ $\mathrm{TaS}_2$ has been extensively studied due to its various charge-density-wave (CDW) phases. Here, we provide novel insights into the CDW melting in 1-$T$ $\mathrm{TaS}_2$, using time- and angle-resolved photoemission spectroscopy with a momentum microscope at the free-electron laser FLASH in Hamburg. Our near-infrared pump–FEL probe experiment uncovers momentum-dependent conduction-band dynamics and core-level responses, advancing our understanding of ultrafast coupled electronic and structural dynamics.

O 26.7 Tue 12:15 H2

**Developing a versatile fiber-based cathodoluminescence detection system for an ultrafast scanning electron microscope** — •Paul H. Bittorf[1], Filip Majstorovic[1], and Nahid Talebi[1,2] — [1]Institute for Experimental and Applied Physics IEAP, Kiel University, 24118 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

Cathodoluminescence (CL) is emitted when a high-energy electron beam interacts with materials like minerals, semiconductors and plasmonic nanoparticles. Depending on the underlying interaction mechanisms of electrons with the sample this radiation can be coherent or incoherent, where both spectral and temporal statistics can be unraveled for material characterization. Thanks to the high spatial resolution and large spectral excitation bandwidth of the electron beams, we could resolve the spatial far-field distribution of locally probed photonic modes by CL microscopy. Moreover, we combined a commercial scanning electron microscope (SEM) with an ultrafast laser system to obtain a pulsed electron beam via the photoemission process. In addition to the excitation by the pulsed electron beam, a time-delayed laser pulse is focused onto the sample to induce an optical near-field and achieve a time-resolved pump-probe measurement. The interaction properties of electrons with nanostructured matter are analyzed through the emitted CL. Here, we report on technical aspects and the implementation of a multimode fiber-based CL detection system inside an ultrafast SEM and highlight its functionality by performing CL spectroscopy and time correlated single-photon counting.

O 26.8 Tue 12:30 H2

**Ultrafast Electron Diffraction and Microscopy of Structural Phase Transitions at Megahertz Rates** — •Till Domröse[1,2] and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

Control over laser-induced structural phase transformations promises tuning of macroscopic materials properties on femtosecond timescales. Ultrafast electron diffraction (UED) elucidates the spatially averaged evolution of lattice symmetries and phonon populations during the transitions. However, resolving nanoscale structural heterogeneity in these measurements remains challenging due to the reduced brightness of pulsed electron beams. Here, we overcome fundamental limitations in the stroboscopic investigation of structural dynamics in thin material films by UED and ultrafast electron microscopy. A high-coherence electron source offers enhanced momentum resolution in collimated electron nanobeams, while thermally-optimized sample supports enable reversible driving of structural transitions at high duty cycles [1]. Utilizing the associated gain in coherent electron current, we conduct nano-UED investigations of charge-density wave dynamics in layered materials, tomographically reconstructing three-dimensional phase formation kinetics in $1T$-$\mathrm{TaS}_2$ [2], and revealing a femtosecond structural quench in $1T'$-$\mathrm{TaTe}_2$ cycled at a repetition rate of 2 MHz [3].

[1] T. Domröse, *et al.*, arXiv:2410.02310 (2024)
[2] T. Domröse, *et al.*, Nature Materials **22(11)** (2023)
[3] T. Domröse, C. Ropers, Physical Review B **110(8)** (2024)

O 26.9 Tue 12:45 H2

**From Electron-Photon Ghost Imaging Towards Entanglement Certification** — •Alexander Preimesberger[1,2], Sergei Bogdanov[1,2], Phila Rembold[1], Santiago Beltrán-Romero[1,2], Dominik Hornof[1,2], Isobel C Bicket[1,2], Nicolai Friis[1], Elizabeth Agudelo[1], Dennis Rätzel[3], and Philipp Haslinger[1,2] — [1]VCQ, Atominstitut, TU Wien, Vienna, Austria — [2]USTEM, TU Wien, Vienna, Austria — [3]ZARM, University of Bremen, Bremen, Germany

Time-resolved detection of single electrons and their associated cathodoluminescence (CL) photons enables the identification of coincident electron-photon pairs. We recently employed this technique to study the tight momentum correlations generated by coherent CL within a transmission electron microscope [1]. In this contribution, we demonstrate ghost imaging using electron-photon pairs in both near-field and far-field configurations. In photonic quantum optics, the ability to produce such images is used to investigate quantum entanglement in photon pairs [2]. We discuss how to translate this concept to electron-photon states and introduce a robust method to certify and quantify their entanglement using measurements in mutually unbiased bases.

[1] A. Preimesberger et al., arXiv:2409.12216 (2024). [2] R. S. Bennink et al., Phys. Rev. Lett. 92 (2004).

## O 27: Solid-Liquid Interfaces: Reactions and Electrochemistry I

Time: Tuesday 10:30–13:00 Location: H4

O 27.1 Tue 10:30 H4

**Combining electrochemical scanning tunneling microscopy with force microscopy** — •Andrea Auer[1,2] and Franz J. Giessibl[2] — [1]Institute of Physical Chemistry, University of Innsbruck, Austria — [2]Institute of Experimental and Applied Physics, University of Regensburg, Germany

Atomic force microscopy (AFM), which can be performed simultaneously with scanning tunneling microscopy (STM) using metal tips attached to self-sensing quartz cantilevers (qPlus sensors) [1], has advanced the field of surface science by providing unprecedented spatial resolution under ultra-high vacuum conditions. The simultaneous performance of AFM and STM with atomic resolution in an electrochemical cell offers new possibilities for local imaging of electrode structures. Here, we present a combined AFM/STM instrument realized with a qPlus sensor and a custom-built potentiostat for electrochemical applications. Graphite was atomically resolved in both STM and AFM channels in acidic electrolytes [2]. The difference in contrast between AFM and STM images demonstrate the ability to measure conductance at the Fermi level (STM) but also the total charge density (AFM) in an electrochemical environment. This allows us to study important electrode processes that involve a change in charge density, such as adsorption, intercalation, or oxidation processes, and their atomic contrasts in more detail.

[1] F.J. Giessibl, Rev. Sci. Instrum. 90, 011101 (2019). [2] A. Auer, B. Eder and F.J. Giessibl, J. Chem. Phys. 159, 174201 (2023).

O 27.2 Tue 10:45 H4

**Small change huge effect – Tuning CO2 reduction to Formaldehyde** — •Michael Busch — Luleå University of Technology, Luleå, Sweden

$CO_2$ reduction is a central technology for energy conversion and as access route to basic feedstock for the chemical industry. Unfortunately, its potential is still hindered by high overpotentials and low selectivity towards post-CO products. So far, post-CO products can only be accessed reliably either through Cu catalysts or selected single atom catalysts like metal phthalocyanines. Recent experiments indicate, that Co phthalocyanine is even able to form formaldehyde in good yields.[1]

Building on these experiments, we will explore the underlying origin of this surprising finding using density functional theory (DFT) computations.[1,2] Our results indicate, that the pure Co phthalocyanine complex does not show any unexpected selectivity. However, upon adjusting potential and pH also the catalyst's protonation state is changed. This minor change in turn shifts the selectivity towards formaldehyde. These surprising insights provide an important puzzle piece for the rational design of improved $CO_2$ reduction catalysts.

[1] A. Singh, M. Busch, M. Robert et al. *J. Am. Chem. Soc.* **146** (2024) 22129.

[2] R. Khakpour, K. Farshadfar, M. Busch et al. *J. Phys. Chem. C.* **128** (2024) 5867.

O 27.3 Tue 11:00 H4

**Quantitative Modeling of the Coordination and Solvation Dynamics of Electrically Charged Solvated Systems via Molecular Dynamics Simulations** — •Zhenyu Wang, Mira Todorova, Christoph Freysoldt, and Jörg Neugebauer — Max Planck Institute for Sustainable Materials

Chemical and biological processes in water are influenced by the dynamics of the water solvation shell of ions. Despite progress in understanding ion solvation dynamics, the structural changes in the solvation shell with varying charge states remain underexplored. This study uses atomistic molecular dynamics calculations to investigate the solvation shell of a Na ion, as a prototype model, focusing on changes in water molecule arrangement due to charge variations. Gaussian process regression is used to analyze the reorientation of $H_2O$ molecules as the Na-ion charge is changed from negative to positive. Results show significant effects of the ionic charge on the coordination to neighboring water molecules, which form distinct polyhedral structures, such as tetrahedra, triangles, pyramids, and octahedra. These formed patterns can be effectively characterized by using the $H_2O$-$H_2O$ distance and $H_2O$-$H_2O$-$H_2O$ angle. At the highest positive charge, $H_2O$ molecules form an octahedral configuration, transitioning to pyramidal and triangular bipyramidal structures as the charge decreases. At a neutral charge, the solvation shell reveals maximum dispersion, which transitions into a single cluster at negative charges. This study provides valuable insights into ion solvation behavior and significantly enhances the understanding of ion solvation dynamics in aqueous environments.

O 27.4 Tue 11:15 H4

**Field-induced water autoionization in two- and three-dimensions** — •Yair Litman and Angelos Michaelides — University of Cambridge, Cambridge, U. K.

The behaviour of water under an electric field critically influences the performance of numerous energy conversion and storage devices and remains a subject of active investigation. Recent experiments have shown that at electric field strengths exceeding $10^8$V/Å, the water dissociation reaction ($2H_2O \rightleftharpoons H_3O^+ + OH^-$) is significantly accelerated, a phenomenon known as the (secondary) Wien effect [1].

In this work, we employ the modern theory of polarization to perform (periodic) *ab initio* molecular dynamics simulations of water under external electric fields, both in bulk and under nanoconfinement. Our simulations reveal that electric fields facilitate the water dissociation reaction by not only reducing the enthalpy of the reaction but also by increasing the corresponding entropic contribution. Furthermore, we demonstrate that geometric constraints imposed by a 2D confinement can amplify the field-induced reaction rates. These findings highlight the importance of entropy changes in field-induced aqueous reactions and propose nanoconfinement as a promising avenue for enhancing the efficiency of electrocatalytic reactions.

[1] J. Cai. *et al.*, Nat. Commun **13**, 5776 (2022)

O 27.5 Tue 11:30 H4

**Predicting Electrocatalytic Urea Synthesis Using a Two-dimensional Descriptor** — •Amy Wuttke and Alexander Bagger — Department of Physics, Technical University of Denmark

Electrochemical synthesis routes offer a sustainable alternative to conventional fossil-based processes for producing chemical commodities. An example is the crucial fertiliser urea ($CO\,(NH_2)_2$), that can be synthesised by co-reducing $CO_2$ and nitrite ($NO_2^-$) on transition metal surfaces [1]. This reaction also serves as a model system for studying electrochemical CN-coupling. However, achieving high selectivity toward urea remains a significant challenge due to the complexity of competing reaction pathways.

In this talk, a predictive framework for urea selectivity is presented based on adsorption energies as descriptors without referring to a full reaction mechanism [2]. Using Density Functional Theory, we calculated 10 adsorption energies as potential descriptors on 19 transition metal surfaces. Through Principal Component Analysis, this high-dimensional dataset is reduced to two key descriptors: *H and *O adsorption energies. Our findings demonstrate that these descriptors effectively explain urea selectivity on transition metals, offering a simplified approach to guide catalyst design.

[1] M. Shibata et al., J. Electrochem. Soc., 145(2), 595-600 (1998), doi: [10.1149/1.1838309].

[2] A. Wuttke and A. Bagger, Predicting Electrocatalytic Urea Synthesis Using a Two-Dimensional Descriptor, in review. Research Square Preprint, Jul. 17, 2024, doi: [10.21203/rs.3.rs-4749942/v1].

O 27.6 Tue 11:45 H4

**Effect of water on the diffusion barriers of $S_{ad}$ on Cu(100) and Ag(100): DFT-calculations** — •Falk Wendorff, Sönke Buttenschön, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Diffusion of adatoms at the electrochemical interface is affected by the electrolyte in various ways. Here we focus on the effect of pure water at the pzc on the diffusion barriers within Transition State Theory. Due to the dynamics of the $H_2O$ molecules in liquid water the process is complicated to simulate. We have investigated the diffusion of a sulfur adatom on Cu(100) and Ag(100) surfaces in the presence of water using explicit water molecules in DFT simulations. The calculations have been carried out with PWscf and PWneb from Quantum ESPRESSO [1]. We have started from initial water layers generated by the Water Structure Creator by Dávila López *et al.* [2] and performed subsequent MD simulations of the water molecules at fixed sulfur and substrate positions. The results show that water lowers the diffusion barriers of sulfur on the metal surfaces compared to the interface versus vacuum.

Funded by the Deutsche Forschungsgemeinschaft project 504552981.

[1] P. Giannozzi *et al.*, J. Phys. Condens. Matter **21**, 395502 (2009), *ibid.* **29**, 465901 (2017).

[2] A. C. Dávila López *et al.*, J. Chem. Phys. **155**, 194702 (2021).

**Invited Talk** O 27.7 Tue 12:00 H4

**Ultrafast electrochemistry beyond the RC time constant** — •Yujin Tong — Universität Duisburg-Essen, Duisburg

Electrochemistry relies on charge transfer, which can occur on time scales from femtoseconds to seconds or longer. Traditional electrochemical detection methods are limited in their ability to study ultrafast processes such as solvent reorganization and electron tunneling. This presentation focuses on the advancements and challenges in ultrafast electrochemistry, specifically exploring processes occurring on timescales shorter than the RC time constant. Traditional electrochemical processes have typically been studied over longer timescales, often constrained by limitations in mass diffusion and hardware capabilities. However, recent developments in ultrafast laser technology and femtochemistry have enabled the observation of rapid processes with femto /pico second time resolution at electrochemical interfaces, such as ultrafast potential relaxation in electric double layers and the dynamics of solvated electrons [1-3]. [1] G. Zwaschka, F. Lapointe, R. K. Campen, Y. Tong, Curr. Opin. Electrochem. 29, 100813 (2021) [2] F. Lapointe, M. Wolf, R. K. Campen, Y. Tong, J. Am. Chem. Soc. 142, 18619-18627 (2020) [3] Z. Huang, M. Bridger, O. A. Naranjo-Montoya, A. Tarasevitch, U. Bovensiepen, Y. Tong, R. K. Campen, arXiv preprint, doi: 10.48550/arXiv.2304.06684 (2023)

O 27.8 Tue 12:30 H4

**Deciphering the Capacitance of the Pt(111)/Water Interface: A Micro- to Mesoscopic Investigation by AIMD and Implicit Solvation** — •Lang Li, Karsten Reuter, and Nicolas Hörmann — Fritz-Haber-Institut der MPG, Berlin

We use *ab initio* molecular dynamics simulations based on density-functional theory to revisit the enigmatic capacitance peak of the electrified Pt(111)/water interface around the potential of zero charge. We demonstrate that counterbalancing the electronic excess charges with partially charged hydrogen atoms constitutes a computationally efficient approach to converged interfacial water structures. The thus enabled detailed analysis of the interfacial water response clarifies that the peak in the capacitance is predominantly due to structural reorientation, although its magnitude is significantly increased by strong internal electronic polarization, also known as charge transfer (CT). We find that CT is more complex than previously thought, resulting from the interplay between chemisorbed water and depolarization effects from surrounding water. Finally, we demonstrate that quantitative agreement with the experimental peak can be achieved through inclusion of the interfacial response into an implicit solvent model for the extended part of the double layer. This suggests that such models can accurately reproduce screened interfacial fields as a function of potential, despite their notoriously small native capacitance. [1] L. Li, K. Reuter, N. G. Hörmann, accepted by ACS Electrochem.

O 27.9 Tue 12:45 H4

**Efficient periodic density functional theory calculations of charged molecules and surfaces using Coulomb kernel truncation** — •Sudarshan Vijay[1], Martin Schlipf[1], Henrique Miranda[1], Ferenc Karsai[1], Martijn Marsman[1], and Georg Kresse[1,2] — [1]VASP Software GmbH, Berggasse 21, 1090 Vienna, Austria — [2]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Kolingasse 14-16, A-1090 Vienna, Austria

Density functional theory (DFT) calculations of charged molecules and surfaces are critical to applications in electro-catalysis. Periodic DFT implementations such as the Vienna ab-initio Simulation Package (VASP) compute the electrostatic potential under 3D periodic boundary conditions, which necessitates charge neutrality. In this work, I will discuss our recent implementation of 0D and 2D periodic boundary conditions. Unlike 3D boundary conditions, our implementation allows for calculations of charged molecules and surfaces. We implement these boundary conditions using the Coulomb kernel truncation method. We compute the electrostatic potential under 0D and 2D boundary conditions by selectively subtracting unwanted long range interactions from the potential under 3D boundary conditions, removing the need for performing any Fourier transforms in padded supercells. To illustrate the computational efficiency of our method, we perform large supercell calculations of the formation energy of a charged chlorine defect on an NaCl(001) surface and perform long time-scale molecular dynamics simulations on an Au(211) | water electrode-electrolyte interface.

## O 28: Graphene: Electronic Structure and Excitations (joint session O/HL)

Time: Tuesday 10:30–12:15 Location: H6

O 28.1 Tue 10:30 H6

**Doping of epitaxial graphene by proximitized 2D quantum islands** — •Julian Koch[1], Sergii Sologub[1,2], Chitran Ghosal[1], Dorothee Boesler[1], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Reichenhainerstr. 70, 09126 Chemnitz — [2]Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv

The effects of 2D quantum islands on the transport properties of monolayer graphene/SiC(0001) were investigated by magnetotransport. Two types of adsorbates are compared, Bi(110) and Pb(111) islands with average coverages of up to 3.6 bilayers (BL) and 3 monolayers (ML), respectively. The analysis is supported by structural investigations using SPA-LEED and STM. The doping behaviour of both materials is fundamentally different. In the case of Bi, the carrier concentration determined from the SdH oscillations remains at $1 \times 10^{13}\ \mathrm{cm^{-2}}$ independent of the Bi coverage, although photoemission spectroscopy revealed a strong doping of the graphene by Bi [1]. This strongly indicates a highly anisotropic carrier concentration across the surface and is confirmed by a positive, temperature independent contribution to the magnetoresistivity. The Bi islands rather behave as antidots and reduce the charge carrier mobility slightly from around 2250 $\mathrm{cm^2/(Vs)}$ for MLG to 1920 $\mathrm{cm^2/(Vs)}$ at 2.4 BL Bi. In contrast, there are no signs of an anisotropic carrier concentration or mobility when Pb is adsorbed. The electron concentration increases uniformly by approximately $5 \times 10^{11}\ \mathrm{ML^{-1}cm^{-2}}$. The mobility is reduced from around 1400 $\mathrm{cm^2/(Vs)}$ for MLG to 1200 $\mathrm{cm^2/(Vs)}$ at 3 ML Pb.

[1] Gierz et al. *Nano Lett.* **8**, 12, 4603 (2008)

O 28.2 Tue 10:45 H6

**Photocurrent control in a graphene-based Floquet topological insulator** — •Weizhe Li[1], Daniel Lesko[1], Tobias Weitz[1], Simon Wittigschlager[1], Christian Heide[1,2], Ofer Neufeld[3], and Peter Hommelhoff[1,4] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — [2]Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA, USA — [3]Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Haifa, Israel — [4]Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München

Topological insulators offer unique opportunities for novel electronics and quantum phenomena. However, intrinsic material limitations often restrict their applications and practical implementation. A circularly-polarized laser pusle can generate topologically non-trivial non-equilibrium states known as Floquet topological insulators (FTIs) which host a variety of topological phenomena. Floquet engineering with strong optical fields opens routes to optically tunable band structures and devices for petahertz electronics.

Here we demonstrate coherent control of photocurrents in lightdressed graphene. Circularly-polarized laser pulses dress the graphene into an FTI, and phase-locked second harmonic pulses drive electrons in the FTI. This approach allows us to measure all-optical anomalous Hall currents and photocurrent circular dichroism, which put FTIs on equal footing with equilibrium topological insulators. The coherent control of photocurrents in graphene-based FTI connects optics tools to condensed matter physics.

O 28.3 Tue 11:00 H6

**Electronic structure of intercalated epitaxial graphene: A first principles study** — •Andres Unigarro[1], Florian Günther[2], Philip Schädlich[1], Bharti Matta[3], Philipp Rosenzweig[3], Kathrin Küster[3], Ulrich Starke[3], Thomas Seyller[1], and Sibylle Gemming[1] — [1]Institute of physics, TU Chemnitz, Chemnitz, Germany — [2]UNESP, Rio Claro, Brazil — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart

Two-dimensional materials such as graphene are fascinating because they combine unique mechanical and electronic properties. The next level of complexity, however, comprises the assembly of various stacked 2D materials to generate structures with desired properties. Intercalation of epitaxial graphene systems is an effective method to tailor the electronic, optical, and transport properties of graphene while keeping its honeycomb lattice on SiC. Furthermore, intercalation facilitates the synthesis of otherwise unstable 2D layers. A wide range of elements have been used as intercalants below a graphene sheet, forming often well-defined heterobilayers with different functionalities. In particular, intercalation of heavy elements such as Pb and Bi are specially promising since they can introduce additional effects such as spin-orbit coupling to the electron gas of graphene and Rashba spin polarization. Using first-principles methods, we investigate the modifications in the electronic structure of epitaxial graphene due to proximity effects induced by intercalation.

O 28.4 Tue 11:15 H6

**Accelerated Exploration of Defective Graphene Superstructures** — •Benedict Saunders[1], Lukas Hörmann[1,2], and Reinhard Maurer[1,2] — [1]Department of Chemistry, University of Warwick, Coventry — [2]Department of Physics, University of Warwick, Coventry

Graphene has been meticulously studied due to its remarkable mechanical, electrical, and thermal properties. It is well documented that introducing various dopants and defects to the lattice can be used to tune the material's properties for a specific application, such as in electronics, sensors, or catalysis. In order to design graphene with specific properties, one must achieve precise control over the composition and concentration of defects. This requires a fundamental understanding of the stability of defects and their interaction in a given superstructure. We present a comprehensive method for exploring the configurational space of defective 2D superstructures. We have extended the SAMPLE structure search code to defects in 2D materials. SAMPLE uses Bayesian learning based on sparse Density Functional Theory data for structure exploration. We show the capabilities of our approach for a proof-of-principle application on free-standing graphene with heteroatom defects. Finally, we use the SAMPLE code to gain physical insight into the interactions between these defects, paving the way for effective and rational growth models of topologically designed defective graphene.

O 28.5 Tue 11:30 H6

**Polymorphism of a two-dimensional Pb layer underneath charge neutral graphene on SiC** — •Markus Gruschwitz, Sergii Sologub, Zamin Mamiyev, Chitran Ghosal, and Christoph Tegenkamp — Institut für Physik, TU Chemnitz, Germany

Since the first studies on graphene, researchers strive to implement its unique properties in industrial relevant processes. The intercalation of epitaxially grown buffer layers on SiC results in high quality, quasi-freestanding graphene, which allows the electronic properties to be modified by varying the intercalants and their arrangement. Pb recently sparked a great interest by reliably providing almost perfectly charge neutral graphene. The Pb layer effectively screens the substrate induced doping. In a novel approach using differential phase contrast in cross-sectional scanning transmission electron microscopy we reveal their vertical charge density distribution. Surprisingly, the charge neutrality is robust against variations in the Pb interface reconstruction. Depending on the preparation, a Pb monolayer often reconstructed in two coexisting phases, the so-called stripe [1] or bubble [2] phase. Intercalated multilayers reveal a similar striped phase arising from two twisted plumbene layers [3]. Here we combine structural investigations by scanning tunneling microscopy and high-resolution low-energy electron diffraction in a model of flexibly arranged grain boundaries releasing lattice mismatch stress.

[1] Materials 14, 7706 (2021), [2] Adv. Mater. Interfaces 10, 2300471 (2023), [3] Phys. Rev. Lett. 129, 116802 (2022)

O 28.6 Tue 11:45 H6

**Facet-dependent growth and properties of graphene on $Al_2O_3$ surfaces from first principles** — •Armin Sahinovic and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

The direct growth of graphene on functional substrates such as sapphire ($Al_2O_3$) enables the use in optoelectronic devices without the necessity of sample transfer. We explore the role of the surface orientation of $Al_2O_3$ on the growth of graphene [1] using density functional theory. The stoichiometric terminations are identified as the most stable surface terminations of the C-, R- and A-plane facets in the framework of *ab initio* thermodynamics. Next, we consider the adsorption of carbon atoms on the different surface facets, varying their position and concentration. The adsorption energy shows the weakest binding at the R-plane and the most favorable at the A-plane. We associate this with the more unsaturated oxygen bonds at the A-plane compared to the R- and C-plane. Furthermore, we explore the graphene - $Al_2O_3$ interaction and its impact on the electronic properties of graphene. Our results provide a deeper understanding of the role of the surface facets of the substrate in the scalable graphene growth on $Al_2O_3$.

Funding by GRK2803 2D-MATURE (Project P4) and computational time at the supercomputers MagnitUDE and AmplitUDE are gratefully acknowledged

[1] Y. Ueda et al., Appl. Phys. Lett. 1, 115 (1), 013103 (2019)

O 28.7 Tue 12:00 H6

**Enhanced light-matter interactions via Sn nanoislands on epitaxial graphene** — •Zamin Mamiyev, Narmina Balayeva, Dietrich R.T. Zahn, and Christoph Tegenkamp — Institut für Physik, Technische Universität Chemnitz

Surface-enhanced Raman scattering (SERS) is an advanced technique for coupling light into quasiparticle excitations in low-dimensional materials, offering promising applications in trace detection, enhanced light-matter interactions, photonic energy harvesting, and catalytic processes. Recent studies in this field have focused on integrating noble metal nanostructures with graphene.

In this study, we investigate a novel SERS platform utilizing tin (Sn) nanoislands to enhance graphene Raman signals by up to two orders of magnitude. We examine the SERS performance on Sn-intercalated charge-neutral and intrinsically doped epitaxial monolayer graphene (MLG) on SiC(0001). The increase in the Raman cross-section and enhanced intensity is accompanied by spectral shifts, which may be correlated with the localized surface plasmons (LSPs) of Sn nanoislands as well as dynamic charge transfer between the Sn particles and graphene. This dynamic charge redistribution, primarily determined by the doping concentration and interface interactions, enables control over the SERS response. Additionally, plasmonic and thermalization-induced carrier density propagation across $\mu m$ ranges indicates efficient coupling between localized and propagating plasmons.

[1] Z. Mamiyev and C. Tegenkamp, 2D Materials. 11, 025013 (2024)
[2] Z. Mamiyev and C. Tegenkamp, Surf. & Int. 34, 102304 (2022)

# O 29: 2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)

Time: Tuesday 10:30–13:00 Location: H8

O 29.1 Tue 10:30 H8

**Line-moiré phases of an epitaxial honeycomb monolayer AgTe/Ag(111)** — •Romana Ganser, Muthu P. T. Masilamani, Begmuhammet Geldiyev, Maximilian Ünzelmann, and Friedrich Reinert — Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

We present angle-resolved photoemission spectroscopy (ARPES) measurements on tunable one-dimensional moiré phases of an epitaxial honeycomb monolayer AgTe/Ag(111) [1]. In this model system, the moiré structure can be tuned almost continuously in contrast to hardly controllable twist angles in bilayer van-der-Waals heterostructures [2]. We experimentally observe moiré minibands and band gaps of 120 - 170 meV suggesting sizable superlattice potentials. By comparing the experimental data to simple model calculations, we analyze the local character of the potential. This provides important information of interface hybridization effects on the band structure, which may not be limited to the system at hand but rather a broad range of moiré interfaces.

[1] Ünzelmann, M. et al. PRL. 124, 176401 (2020).
[2] Lisi, S. et al. Nat. Phys. 17, 189-193 (2021).

O 29.2 Tue 10:45 H8

**Photoemission Time Scale Determination: the Effect of Crystal Dimensionality and Electronic Correlation** — •Fei Guo[1], Dmitrii Usanov[2], Eduardo B. Guedes[2], Mauro Fanciulli[3], Arnaud Magrez[1], Michele Puppin[1], and Hugo Dil[1,2] — [1]Institute of Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Photon Science Division, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Laboratoire de Physique des Matériaux et Surfaces, CY Cergy Paris Université, Cergy-Pontoise, 95031, France

Spin polarization of photoelectrons from spin-degenerate dispersive initial states originates from the interference of multiple photoemission channels, measuring the spin polarization with spin- and angle-resolved photoemission spectroscopy (SARPES) allows the estimation of the phases of the interfering channels, and hence the Eisenbud-Wigner-Smith (EWS) time delay of photoemission, which is the amount of time required by the photoelectron to evolve into a free particle final state. While not directly measurable for solid-state photoemission, this time scale has been measured for gaseous photoionization, which is generally in the attosecond (10^-18s) range.

We present investigations with multiple materials of different properties, and by comparing with previous studies, we propose a relationship between the EWS time delay, electronic correlation mechanism, and dimensionality.

O 29.3 Tue 11:00 H8

**Disorder effects in the Band Structure of Transition Metal Dichalcogenide alloys $A_xB_{1-x}Se_2$ (A, B= Cr, Mo, W)** — •Sarath Sasi[1], Aki Pulkkinen[1], Laurent Nicolaï[1], Raphaël Salazar[1], Christine Richter[2,3], Karol Hricovini[2,3], and Ján Minár[1] — [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

Recent advances in materials synthesis have enabled the creation of 2D TMDC alloys, which offer unique opportunities for tailoring electronic and optoelectronic properties to meet diverse application demands.[1].This study investigates the band structure evolution of $A_xB_{1-x}Se_2$ alloys (A, B = Cr, Mo, W) across varying composition fractions ($x$). Using the Coherent Potential Approximation (CPA)[2], which accurately models scattering in disordered systems, theoretical calculations were performed with the *SPR-KKR* package[3]. Results reveal that some of the TMDC alloys maintain their band structures without significant disorder effects. Angle-Resolved Photoemission Spectroscopy (ARPES) measurements align closely with one-step model photoemission calculations, confirming theoretical predictions. These insights provide a foundation for tailoring electronic properties, advancing their applicability in next-generation devices.

[1] Zhou, J., Lin, J., Huang, X., et al. Nature, 556, 355-359 (2018).
[2] Soven, P., Phys. Rev., 156, 809(1967).
[3] Braun, J., Minar, J., Ebert, H. Physics Reports, 740 (2018).

O 29.4 Tue 11:15 H8

**Unveiling Doping-Induced Electronic Modifications in Antiferromagnetic MPS$_3$ van der Waals Materials** — •Till Willershausen[1], Jonah Elias Nitschke[1], Patrick Merisescu[2], David Janas[1], Lasse Sternemann[1], Michele Capra[1], Mira Arndt[1], Valentin Mischke[1], and Mirko Cinchetti[1] — [1]TU Dortmund University — [2]Bath University

Antiferromagnetic van der Waals (vdW) materials, with scalability to monolayer thickness, semiconducting properties, and intrinsic antiferromagnetic ordering, hold promise for spintronic and quantum technology applications. We investigate alkali metal doping effects on the MPS$_3$ family (M = Mn, Ni, Co, Fe) of 2D antiferromagnetic vdW materials, revealing doping-induced changes in their electronic structure. X-ray Photoelectron Spectroscopy (XPS) shows shifts in oxidation states in NiPS$_3$, CoPS$_3$, and FePS$_3$, while MnPS$_3$ displays no significant changes, indicating distinct charge transfer. Further investigation with Angle-Resolved Photoelectron Spectroscopy (ARPES) reveals new alkali-metal induced bands appearing above the previous valence band maximum. This analysis highlights doping-induced modifications and contrasts in transition metal behavior in MPS$_3$, providing insights into doping mechanisms and electronic tunability.

O 29.5 Tue 11:30 H8

**Enhanced electron-phonon coupling in few-layer MoTe$_2$ from micro-ARPES** — •Thomas P. van Waas[1], Julia Issing[2], Marco Gibertini[3], Christophe Berthod[2], Anna Tamai[2], Felix Baumberger[2,4], and Samuel Poncé[1,5] — [1]European Theoretical Spectroscopy Facility, Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium — [2]Department of Quantum Matter Physics, University of Geneva, Switzerland — [3]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, University of Modena and Reggio Emilia, Italy — [4]Swiss Light Source, Paul Scherrer Institut, Switzerland — [5]WEL Research Institute, Belgium

Bulk orthorhombic T$_d$-MoTe$_2$ is a type-II Weyl semimetal with a superconducting critical temperature of $T_c = 0.1$ K. Transport measurements show a monotonic increase in $T_c$ as the thickness of multilayer MoTe$_2$ is reduced, reaching $T_c = 7.6$ K in the monolayer. We investigate photoemission kinks in the electron pocket of exfoliated mono- bi-, and trilayer MoTe$_2$ from micro-focused angle-resolved photoemission spectroscopy. We use a custom code to quantify the electron self-energy $\Sigma_n(E)$ for a parabolic non-interacting dispersion, and obtain from $\Sigma_n(E)$ the Eliashberg spectral function $\alpha^2F_n(\omega)$ using the maximum entropy method. We find two dominant phonon modes in $\alpha^2F_n(\omega)$ for the mono- and trilayer, with a large enhancement of the lower-frequency phonon mode in the former. We also provide tentative results for the bilayer, where quantification is more challenging due to a small splitting of the electronic bands.

O 29.6 Tue 11:45 H8

**Electronic structure of V-doped WSe$_2$** — •Jana Kähler[1,2], Florian K. Diekmann[1,2], Matthias Kalläne[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 — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics represents a promising and energy-efficient alternative to conventional electronics, with significant potential applications, e.g., in areas such as classical and quantum computing. The vanadium-doped layered transition metal dichalcogenide 2$H$-WSe$_2$ is a promising candidate to fulfill the desired properties as a room-temperature magnetic semiconductor with gating tunability. Here, we present a comprehensive electronic structure study of chemical vapor transport-grown pristine and V-doped WSe$_2$ by soft X-ray, VUV and 11eV-laser ARPES, highlighting the influence of a low V doping concentration on the electronic structure of WSe$_2$.

O 29.7 Tue 12:00 H8

**Unraveling magnetic ordering in a van der Waals correlated**

**material** — Tommaso Pincelli[1,2], •Tania Mukherjee[1,2], Lawson Lloyd[2], Shuo Dong[2,3], Yoav William Windsor[1,2], Martin Wolf[2], Laurenz Rettig[2], and Ralph Ernstorfer[1,2] — [1]Technische Universität Berlin, 10623 Berlin, Germany — [2]Fritz-Haber-Institute of the Max Planck Society, 14195 Berlin, Germany — [3]Beijing National Laboratory for Condensed Matter Physics, China

Layered van der Waals (vdW) materials offer a compelling platform to investigate various emergent quantum properties in low dimensions. $Fe_3GeTe_2$ (FGT), a vdW ferromagnetic metal, is well-known for exhibiting exotic phenomena, ranging from skyrmion formation to heavy fermion behavior. However, an understanding of the magnetic ordering, a key feature for spintronic applications, still remains elusive in this material. In particular, the interplay of both local magnetic moments and an itinerant mechanism in the formation of ferromagnetic ordering in FGT, a non-$f$-electron correlated system, remains to be clarified. Using time- and angle-resolved photoemission spectroscopy (trARPES) and first-principles calculations, we provide evidence for an ordering mechanism in FGT by observing a pronounced reduction in the Stoner exchange gap. This stands in contrast to earlier temperature-dependent ARPES studies of the electronic structure of FGT, which favored a localized excitation model over the weak-coupling itinerant picture. We also observe the impact of phononic excitations which further confirm our findings.

O 29.8 Tue 12:15 H8

**Spin structure of the unoccupied surface state at AgTe/Ag(111)** — •Carolin Benfer, Marcel Holtmann, and Markus Donath — Physikalisches Institut, Universität Münster, Germany

The AgTe/Ag(111) surface alloy has recently been investigated as a model system for the role of orbital angular momentum in the formation of spin effects in the electronic structure [1]. Two $p$-like surface states were detected in ARPES measurements, one shows a Rashba-type spin splitting, while the other one does not. This behavior is attributed to the symmetries of the orbital wave functions of the electrons. For the unoccupied states a third surface state has been predicted. Following the symmetry arguments given in [1], a Rashba-type spin splitting of the state is expected.

We use inverse photoemission (IPE) to directly study the unoccupied state of the surface alloy. Low-energy electron diffraction and scanning tunneling microscopy measurements confirm a homogeneous monolayer film of the surface alloy, which is growing in a honeycomb structure. Angle-resolved IPE measurements detect the predicted surface state with free electron-like dispersion. Spin-resolved IPE measurements reveal a Rashba-type spin structure.

[1] M. Ünzelmann *et al.*, Phys. Rev. Lett. **124**, 176401 (2020)

O 29.9 Tue 12:30 H8

**Orbital mixing as key mechanism for ferromagnetism in van der Waals CrI3** — •Alessandro De Vita[1,2], Srdjan Stavrič[3], Roberto Sant[4], Nicholas B. Brookes[4], Giancarlo Panaccione[5], Silvia Picozzi[3], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1,2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Straße des 17 Juni 135, 10623 Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [3]Consiglio Nazionale delle Ricerche CNR-SPIN, c/o Università degli Studi G. D'Annunzio, 66100 Chieti, Italy — [4]ESRF, The European Synchrotron, 71 Avenue des Martyrs, CS40220, 38043 Grenoble Cedex 9, France — [5]Istituto Officina dei Materiali (IOM)-CNR, Laboratorio TASC, in Area Science Park, S.S.14, km 163.5, I-34149 Trieste, Italy

Van der Waals ferromagnets constitute a versatile platform where exotic quantum states can be realized; among them, CrI3 is a prototypical and widely studied 2D ferromagnet, with promising applications in spin- and orbitronics. Despite that, key information on its electronic occupation and stabilization of the magnetic configuration are missing. By means of complementary absorption and photoemission spectroscopies, and density functional theory calculations, we give a description of the orbital character of bulk CrI3, and demonstrate that the emergence of ferromagnetism in this material is underpinned by the orbital mixing between I p and Cr eg states. Our results have clear impact on the understanding of how microscopic interactions at the orbital level stabilize ordered states in van der Waals ferromagnets.

O 29.10 Tue 12:45 H8

**Resonant Photoemission Studies of Transition Metal Sulfides and Selenides** — •Yashasvi Mehra[1,2,3], Samuel Beaulieu[4], Mauro Fanicullli[1,2], Olivier Heckmann[1,2], Karol Hricovini[1,2], Aki I.O. Pulkkinen[3], Jan Minar[3], and Maria Christine Richter[1,2] — [1]Université Paris-Saclay, CEA, LIDYL, Gif-sur-Yvette, France — [2]CY Cergy Paris Université, CEA, LIDYL, Gif-sur-Yvette, France — [3]University of West Bohemia, NTC, Pilsen, Czech Republic — [4]Universite de Bordeaux CNRS CEA, CELIA, UMR5107, F33405 Talence, France

By performing resonant ARPES measurements and SPR-KKR photoemission calculations on Transition Metal Selenide, Sulfide and the Vanadium intercalated NbS2 systems, we study the interplay between different decay mechanisms in resonant conditions, radiation-less Raman Auger and Classical Auger emissions. Through a method proposed by Cini and Sawatzky we can determine the on-site Coulomb interaction per element in some cases. On the theoretical front the calculations are performed using the SPR-KKR method, which is based on one-step model, that incorporates the effect of all matrix elements which accounts for the photoemission process. Furthermore, we analyze calculated ARPES, XAS, element and orbital resolved band structure underlining agreement with experimental results and helping with its interpretation.

## O 30: Surface Magnetism

Time: Tuesday 10:30–12:45 Location: H11

O 30.1 Tue 10:30 H11

**Spin-polarized chiral edge modes in the topological nodal-point superconductor Mn/Ta(110)** — •Felix Zahner[1], Felix Nickel[2], Roberto Lo Conte[3], Tim Drevelow[2], Roland Wiesendanger[1], Stefan Heinze[2], and Kirsten von Bergmann[1] — [1]University of Hamburg, Germany — [2]University of Kiel, Germany — [3]University of Groningen, The Netherlands

Topological superconducting phases in magnet-superconductor hybrid (MSH) - systems have been investigated recently due to their potential applications in quantum devices. Zero-energy states and chiral edge modes have previously been observed in ferromagnetic 1D [1] and 2D [2] MSH systems. In a 2D antiferromagnet (AFM) MSH and a spin spiral MSH system, gapless topological nodal-point superconducting (TNPSC) phases have been observed [3, 4].

Using scanning tunnelling microscopy/spectroscopy (STM/S), we investigate the mono- and bilayers on a Ta(110) surface. Both exhibit local AFM order and tight-binding calculations indicate that both host a TNPSC phase. Interestingly, we observe edge modes not only at the boundaries between the TNPSC and the topologically trivial superconducting substrate, but also at specific boundaries between these two AFM systems of Mn mono- and bilayer. Our spin-polarized STM measurements reveal a significant spin-polarization of this edge mode, which we discuss based on the tight-binding results.

[1] Nadj-Perge, S. et al., Science 346, 602 (2014). [2] Palacio-Morales, A. et al., Sci. Adv. 5, eaav6600 (2019). [3] Bazarnik, M. et al, Nat Commun 14, 614 (2023). [4] Brüning, R. et al., arXiv:2405.14673.

O 30.2 Tue 10:45 H11

**Interaction of chiral molecules with magnetic substrates: An ongoing DFT puzzle** — •Nicolae Atodiresei — Peter Grünberg Institute (PGI-1), Forschungszentrum Jülich, D-52425 Jülich

A challenging puzzle in surface science that has to be solved is the interplay between electron spin and molecular chirality. As an example, the interaction of chiral helical aromatic molecules with magnetic surfaces leads to an enantioselective adsorption, i.e. molecules of opposite handedness would preferentially adsorb to ferromagnetic islands with opposite magnetization [1]. In this talk, I will discuss how state-of-the-art spin-resolved *ab initio* simulations based on density functional theory calculations support and guide the interpretation of scanning tunneling microscopy experiments performed on the adsorption of heptahelicene molecule onto ferromagnetic cobalt islands.

The author acknowledges funding from CRC 1238 of the Deutsche Forschungsgemeinschaft and computing time granted on the supercomputer JURECA at Forschungszentrum Jülich.

[1] Mohammad Reza Safari et al., Adv. Mater. **36**, 2308666 (2024)

O 30.3 Tue 11:00 H11

**Spin-lattice relaxation of nitrogen-vacancy centers in nanodiamonds on conducting and non-conducting surfaces** — •Izidor Benedičič[1], Yuri Tanuma[1], Bastien Anézo[1,2], Žiga Gosar[1,3], and Denis Arčon[1,3] — [1]Department of Condensed Matter Physics, Jožef Stefan Institute, Ljubljana, Slovenia — [2]Institut des Matériaux de Nantes Jean Rouxel (IMN), Nantes University, Nantes, France — [3]Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia

Nitrogen-vacancy (NV) centers in diamond are versatile probes for the detection of both static magnetic fields and magnetic fluctuations. While single-NV sensors are very capable, they suffer from high cost and experimental complexity. Nanodiamonds with embedded NV ensembles offer a promising low-cost alternative, however, their application in solid-state physics has been largely overlooked. Here, we investigate the use of nanodiamonds for measuring the electrical conductivity of substrates. We measured the temperature dependence of longitudinal relaxation time $T_1$ of NV centres in nanodiamonds on glass and gold substrates. We find that $T_1$ is determined both by phononic relaxation processes and the coupling to the magnetic moments at the surface. All samples show a stretched exponential relaxation, hinting at a significant distribution of relaxation processes. The theoretical models show the intrinsic distribution is too wide to reliably detect coupling to electronic states even of very good conductors. Our results hint at the limitations of nanodiamonds for measurements of transport properties in condensed matter systems.

O 30.4 Tue 11:15 H11

**Imaging in-plane magnetic domains using magnetic circular dichroism in darkfield laser PEEM** — •David Huber[1], Friederike E. Wührl[1], Frank O. Schumann[2], and Wolf Widdra[1] — [1]Martin-Luther-Universität Halle-Wittenberg — [2]Max-Planck-Insitut für Mikrostrukturphyisk, Halle

Magnetic circular dichroism (MCD) in threshold photoelectron emission microscopy (PEEM) enables imaging of magnetic domains at the nanoscale. Utilizing femtosecond (fs) laser excitation in a laboratory setting offers a significant advantage in terms of temporal resolution compared to more commonly used X-ray MCD measurements. However, this poses new challenges with respect to in-plane magnetization, given the previously reported low domain contrast [1, 2].

In this contribution we show that symmetry breaking and photoelectron filtering in momentum and energy help to overcome these challenges. Using this methodology, we obtain MCD contrast for in-plane domains of 11 nm Fe(001)-(1 × 1)-O on MgO(001) using both continuous wave and fs laser excitation at normal incidence and compare these results to a Fe(001)-(1 × 1)-O single crystal in PEEM and $\mu$ARPES.

[1] Marx et al., PRL **84**, 5888 (2000).

[2] Nakagawa et al. PRL **96**, 237402 (2006).

**Invited Talk** O 30.5 Tue 11:30 H11

**Resonant molecular transitions in femtosecond second harmonic generation spectroscopy of Fe-porphyrin/Cu(001)** — •Andrea Eschenlohr[1], Rui Shi[2], Jinghao Chen[1], Ping Zhou[1], Uwe Bovensiepen[1], Wolfgang Hübner[2], and Georg Lefkidis[2] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Department of Physics, RPTU, Box 3049, 67653 Kaiserslautern, Germany

Metal-organic molecular adsorbates on metallic surfaces are potential future materials for (spin-)electronics applications, provided that the molecule-substrate interaction can be analyzed and manipulated in a targeted manner. By combining interface-sensitive optical second harmonic generation (SHG) spectroscopy experiments and electronic structure calculations using coupled cluster methods including optical excitations on iron-octaethylporphyrin (FeOEP) adsorbed on Cu(001), we find that the SHG response of FeOEP/Cu(001) is modified at 2.15-2.35 eV fundamental photon energy compared to the bare Cu(001) surface. We conclude a resonantly enhanced SHG by molecular transitions, which results from a strong charge-transfer character of the molecule-substrate interaction [1]. Pump-probe SHG reveals a markedly slower relaxation time at this resonance, indicating an increased lifetime of the optically induced state compared to the bare Cu(001) surface, which will be discussed in the context of charge transfer dynamics.

[1] Eschenlohr et al., arXiv:2409.09801

O 30.6 Tue 12:00 H11

**Single-layer magnetism of epitaxial NiBr2 and FeBr2 on NbSe2** — •Sebastien E. Hadjadj[1], Carmen Gonzalez-Orellana[2], Adriana Candia[3], Pierluigi Gargiani[4], Matthias Muntwiler[5], Jan Dreiser[5], Jorge Lobo[3], Celia Rogero[2], and Maxim Ilyn[2] — [1]Materials Physics Center (MPC), Donostia, Spain — [2]Centro de Fisica de Materiales (CSIC/UPV-EHU), Donostia-San Sebastian, Spain — [3]Instituto de Nanociencia y Materiales de Aragon (INMA),Zaragoza, Spain — [4]ALBA Synchrotron Light Source, Barcelona, Spain — [5]Paul Scherrer Institut, Villigen, Switzerland

Two-dimensional metal dihalides exhibit promising magnetic and electronic properties. Over the past years, the research focus on novel 2D magnetic materials has shifted to transition metal di-halides (TMDH). Recent reports have shown that the first layer of Br-based TMDH grown on Au(111) behaves structurally and magnetically differently from the second layer [1-2]. Here we report the first layer growth of NiBr2 and FeBr2 on NbSe2, which shows no signs of decomposition as observed for NiBr2 on Au(111) and shows unaffected stable magnetic properties ranging from monolayer to multilayer. The structural characterization of the samples revealed a strong temperature dependence in the resulting island growth and appearence of the moiré pattern. XMCD measurements probed magnetic ordering down to the 2D limit, which is in agreement with the literature values. In the case of FeBr2 a strong reduction of the spin magnetic moment has been observed. [1] Djuro Bikaljevic et al., ACS Nano, 15, 14985, (2021) [2] S. E. Hadjadj et al., Chem. Mater., 35, 23, 9847-9856, (2023)

O 30.7 Tue 12:15 H11

**Graphene intercalated Eu on magnetic surfaces a DFT study** — •Gustav Bihlmayer[1], Polina M. Sheverdyaeva[2], Matteo Jugovac[3], Luisa Ferrari[4], Frederico Mazzola[5], Paolo Perna[6], Nicolae Atodiresei[1], and Stefan Blügel[1] — [1]Peter Grünberg Institute (PGI-1), Forschungszentrum Jülich, D-52425 Jülich — [2]CNR-ISM, 34149 Trieste, Italy — [3]Elettra Sincrotrone Trieste, 34149 Trieste, Italy — [4]CNR-ISM, 00133 Roma, Italy — [5]CNR-IOM, 34149 Trieste, Italy — [6]IMDEA Nanociencia, Campus de Cantoblanco, 28049, Madrid, Spain

Europium can be intercalated between graphene and magnetic surfaces like Co(0001) or Ni(111) forming a $\sqrt{3} \times \sqrt{3}$ layer [1]. The doping of graphene can create a pronounced flat band at the Fermi level and the interaction of the $4f$ states with the $\pi$ band of graphene leads to spin-selective hybridization and opening of the Dirac cone with interesting consequences for edge channels [2]. This system can be compared to Eu on-top of a graphene covered Co substrate, that changes the magnetic coupling between the lanthanide and the substrate [3] and modifies the graphene's interaction with the $4f$ states. Further stacking combinations are possible and will be discussed [4].

We acknowledge funding from the FLAG-ERA grant SOgrapMEM and from CRC 1238 of the Deutsche Forschungsgemeinschaft.

[1] F. Huttmann et al., Phys. Rev. B **95**, 075427 (2017) [2] P. M. Sheverdyaeva et al., Phys. Rev. Lett. **132**, 266401 (2024) [3] M. Jugovac et al., Adv. Mater. **35**, 2301441 (2023) [4] M. Jugovac et al., Carbon **230**, 119666 (2024)

O 30.8 Tue 12:30 H11

**Emergence of Ferromagnetism in 3d-4f Hetero-Bimetallic Surface-Architectures** — •Massine Kelai[1], Serim Jeon[1], Dasom Choi[1], Corina Urdaniz[1], Pierre Josse[1], Jaehyun Lee[1], Stefano Reale[1], Yongwoo Kim[1], Weibin Li[2], Pierluigi Gargiani[2], Woo-Suk Noh[3], Dominik Lungerich[4], Christoph Wolf[1], Fabio Donati[1], and Lucinao Colazzo[1] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea — [2]ALBA Synchrotron Light Source, 08290 Catalonia, Spain — [3]MPPC/CPM, Max Planck POSTECH, Pohang 37673, Republic of Korea — [4]Center for Nanomedicine, Institute for Basic Science (IBS), 50 Yonsei-ro, Seodaemun-gu, 03722 Seoul, Republic of Korea

Surface-confined metal-organic coordination networks (SMONs) are emerging platforms for designing tunable low-dimensional nanostructures, with 3d-4f hetero-bimetallic systems being promising candidates for high-density memory and qubit applications. However, the mechanisms underlying their formation and magnetic interactions remain largely unexplored. Here, we investigate a novel 3d-4f SMON, Dy-FeTCPP (TCPP = 5,10,15,20-(tetra-4-cyanophenyl)porphyrin), formed on Au(111) via on-surface chemical reaction pathways. Using X-ray absorption spectroscopy, magnetic circular dichroism, scanning tunneling spectroscopy, and density functional theory, we show that lanthanide insertion induces strong substrate-mediated ferromagnetic coupling between 3d units, driven by porphyrin core deformation upon Dy-cyanophenyl bonding. This work advances the understanding of SMONs, paving the way for scalable quantum devices on surfaces.

## O 31: Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation II

This focus session aims to discuss recent advances in the on-surface synthesis, manipulation, characterization, and understanding of complex molecular architectures on surfaces. The interest in surface-confined molecular nanostructures emerges from their prospective applications in nanoscale (opto-) electronics, spintronics, solar cells, energy storage devices, and other fields. The bottom-up fabrication of surface-supported nanostructures can be based on molecular self-assembly utilizing non-covalent intermolecular interactions, covalent on-surface synthesis, or the direct manipulation of molecules. Molecular self-assembly usually leads to highly ordered nanostructures, controlled by non-covalent interactions, adsorbate-substrate interactions, as well as thermodynamic and kinetic factors. On-surface synthesis by covalent coupling of reactive precursors adsorbed on metallic, semiconducting, or even insulating surfaces has emerged as a powerful method that has opened new possibilities in exploring new routes towards the synthesis of complex low-dimensional nanostructures with unprecedented material properties, often via novel chemical reactions not available in conventional organic chemistry. Finally, the direct manipulation of molecules with the tip of a scanning probe microscope allows for unprecedented chemical transformations or structural modifications, as envisioned by the pioneers of nanotechnology. This focus session is intended to provide a platform for addressing current trends in these closely linked fields from various perspectives in experiment and theory.

Organized by
Sabine Wenzel (University of Marburg) and Christian Wagner (Forschungszentrum Jülich)

Time: Tuesday 10:30–13:00 Location: H24

O 31.1 Tue 10:30 H24

**AMAN-SPM: Autonomous Molecular and Atomic Nanofabrication via SPM** — •Bernhard Ramsauer[1], Qigang Zhong[2], Bettina Könighofer[3], and Oliver T. Hofmann[1] — [1]Institute 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

The precise manipulation of individual molecules and atoms using scanning probe microscopy (SPM) offers transformative possibilities for nanofabrication. Yet the inherently stochastic nature at the nanoscale and the labour-intensive process of building nanostructures contains significant challenges. In this contribution, we introduce AMAN-SPM, a tool that integrates reinforcement learning and automation to revolutionize the on-surface synthesis process.

AMAN-SPM employs dedicated reinforcement learning agents to optimize the manipulation parameters, which allows for precise positioning, reorientation, and the controlled breaking and formation of molecular bonds. Coupled with machine vision and path-planning algorithms, this system autonomously constructs nanostructures, eliminating the need for human intervention.

Beyond fabrication, AMAN-SPM enhances real-time data acquisition and analysis, providing detailed physical insights into molecular interactions. This establishes a foundation for scalable nanostructures with tailored properties.

O 31.2 Tue 10:45 H24

**Sliding friction over covalent bonds increases with bond order** — Shinjae Nam[1], Lukas Hörmann[2,3], Oliver Gretz[1], Oliver T. Hofmann[2], Franz J. Giessibl[1], and •Alfred J. Weymouth[1] — [1]Universität Regensburg, Regensburg, Deutschland — [2]TU Graz, Graz, Österreich — [3]The University of Warwick, Warwick, U.K.

Friction is governed by atomic-scale interactions, yet we lack a complete understanding of its working at this length scale. To address this, we reduce one sliding surface to the limit of a single atom and measure sliding friction with lateral force microscopy over single bonds. We examine islands of PTCDA on Cu(111), which present a rich variety of covalent and hydrogen bonds. There is a large variety in the maximum energy dissipation over different covalent bonds. The maximum energy dissipation over hydrogen bonds has similar values, although energy dissipation over hydrogen bonds is observed at lower heights than over covalent bonds. With DFT-based simulations and a machine-learning model, we determine that larger bond order is correlated to higher sliding friction.

**Invited Talk** O 31.3 Tue 11:00 H24

**Single molecule machines on surface** — •Francesca Moresco — TU Dresden. Germany

Scanning tunneling microscopy is a unique experimental technique to control the motion of a single molecule, testing the boundary between classical and quantum movement and making thermodynamics at the scale of a single molecule accessible to experimental investigation. Under the tip of a scanning tunneling microscope, inelastic tunneling electrons or local electric fields can produce controlled rotations or translations of a single adsorbed molecule, while thermal excitation can modify the energy barrier for motion. In this talk, we will discuss the controlled rotation and translation of asymmetric and chiral model structures adsorbed on the Au(111) surface.

O 31.4 Tue 11:30 H24

**How to measure cones of reaction for single-molecule collisions** — •Matthew J. Timm[1], Stefan Hecht[2], and Leonhard Grill[1] — [1]Institute of Chemistry, University of Graz, Austria — [2]Department of Chemistry & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Collisions between reagents are necessary for bond formation, and hence fundamental to reaction. The collision outcome depends on the collision energy, which must be enough to overcome the reaction barrier, and on the collision geometry, which modifies the height of this barrier. The collision geometry is defined by the relative orientation of reagents at the point of collision and on the miss-distance between their centers of mass (termed the impact parameter). Selection of impact parameter has been demonstrated for on-surface reactions with a 'surface-molecular-beam' of CF2 'projectiles', formed by dissociation of chemisorbed CF3 molecules with a scanning tunneling microscope tip, aimed along Cu-rows of the Cu(110) surface toward chemisorbed 'targets' [1]. However, control over the relative orientation of the target has remained elusive. Here a singly-debrominated molecular species (BTFyl) is chosen as a target, as it adopts many possible adsorption alignments relative to the incoming CF2 projectile. This allows simultaneous control over both the impact parameter and reagent orientation, thus allowing an unprecedented ability to map how collision geometry contributes to collision outcome.

[1] Anggara, K.; Leung, L.; Timm, M. J.; Hu, Z.; Polanyi, J. C.; Faraday Discuss., 2019, 214, 89-103.

O 31.5 Tue 11:45 H24

**Friction Anisotropy in the Sliding Motion of PMMA microsphere on Rippled PVS Surface** — •Ebru Cihan[1], Hesam Khaksar[2], Kevin Lubig[3], Stephan Gräf[3], Frank A. Müller[3], and Enrico Gnecco[1,2] — [1]TU Dresden — [2]Jagiellonian University — [3]Friedrich Schiller University Jena

The sliding motion of an elastically driven polymethyl methacrylate (PMMA) microsphere on a rippled polyvinyl siloxane (PVS) surface (laser-induced periodic surface structures LIPSS) was investigated for different values of normal load, scan velocity and temperature. The morphologies of the PMMA spheres and modified PVS surfaces were observed to be geometrically convoluted in AFM topographies recorded simultaneously with friction measurements. The spheres were rubbed both parallel and perpendicular to the LIPSS, and the resulting friction was found to be nearly constant, exhibiting a stick-slip behavior over time. This result differs from the reverse stick-slip observed in friction characterizations with similar PMMA microspheres on harder periodic surfaces, such as wedge-shaped silicon gratings [Trib. Lett. 67, 2019] and rippled stainless steel [Appl. Mater. Interfaces 15, 2023]. In both scanning cases, the friction force was found to increase linearly with increasing load, consistent with the increase in contact area expected from Persson contact theory. Furthermore, friction was observed to increase logarithmically with velocity, and to decrease with increasing temperature in accordance with Eyring's reaction rate theory. The stability of this sample system suggests its possible application as a basic unit for artificial tactile sensors.

O 31.6 Tue 12:00 H24

**Electronic and phononic frictional dissipation in single-molecule dynamics at CO-decorated tips** — •Lukas Hörmann and Reinhard J. Maurer — University of Warwick, Coventry, UK

Friction causes significant energy loss in any moving mechanical device. As the miniaturisation of devices reaches the quantum limit, so do dynamical dissipation processes. Fundamentally quantum mechanical mechanisms govern friction at the nanoscale. We account for all relevant quantum mechanical effects, such as charge transfer, or van der Waals interactions, by employing density functional theory, machine learning, and non-adiabatic molecular dynamics. Using this approach, we investigate friction energy dissipation at the natural limit of singular atoms. This allows us to explore how the local electronic and geometric structure affects the dissipation of mechanical energy, where electron-phonon and phonon-phonon coupling give rise to electronic and phononic excitations. Focusing on the example of CO on various Cu surface geometries, we find that electron-phonon coupling strongly depends on the local electronic density of states, while the geometric structure significantly influences phonon-phonon coupling. Our findings quantitatively agree with experiment. Finally, we present a mechanistic interpretation of our findings that provides insights into the underlying physics of single-molecule dynamics on surfaces.

O 31.7 Tue 12:15 H24

**Manipulation of a CO molecule on a copper surface with lateral force microscopy** — •Norio Okabayashi[1], Alfred. J. Weymouth[2], Shinjae Nam[2], Sophia Schweiss[2], Thomas Frederiksen[3,4], and Franz J. Giessibl[2] — [1]School of Mathematics and Physics, Kanazawa University — [2]Institute of Experimental and Applied Physics, University of Regensburg — [3]Donostia International Physics Center — [4]IKERBASQUE, Basque Foundation for Science

The manipulation of a single molecule on a surface by scanning tunneling microscopy (STM) and atomic force microscopy (AFM) has been intensively studied because of its relation to friction research. Recently, we have studied the manipulation process for CO on a Cu(110) surface with AFM, STM and density functional theory [1][2]. We found that at the tip height for the beginning of the manipulation, CO is manipulated from the top to the neighboring top site by transiently using the bridge site, but for lower tip heights, the manipulation occurs from the top to the bridge site and then from the bridge to the neighboring top site. Here, we have extended our experimental technique by incorporating lateral force microscopy, where the tip oscillates laterally [3], to directly observe the energy dissipation during manipulation. Indeed, the observation confirms the validity of our previous claim. This result paves the way for quantitative evaluation of dynamic friction during manipulation. [1] N. Okabayashi, T. Frederiksen, A. Liebig, F. J. Giessibl, Phys. Rev. Lett. 131 (2023) 148001, [2] N. Okabayashi, T. Frederiksen, A. Liebig, F. J. Giessibl, Phys. Rev. B 108 (2023) 165401, [3] A. J. Weymouth, J. Phys.: Condens. Matter 29 (2017).

O 31.8 Tue 12:30 H24

**Intermediates, reactions and products of cyclocarbons** — •Leo Gross[1], Fabian Paschke[1], Florian Albrecht[1], Yueze Gao[2], Igor Roncevic[3], and Harry L. Anderson[2] — [1]IBM Research Europe - Zurich, Rüschlikon, Switzerland — [2]Oxford University, Chemistry Research Laboratory, Oxford, UK — [3]University of Manchester, Department of Chemistry, Manchester, UK

Cyclocarbons, molecular allotropes of carbon in which all carbon atoms are two-fold coordinated, have been synthesized on surface using tip-induced chemistry [1-4], and the formation of larger cyclocarbons by dimerization of precursors was shown [4]. This presentation will focus on products, reactions and intermediates of cyclocarbons, generated by tip-induced chemistry on ultrathin NaCl layers and characterized by STM and AFM with CO-functionalized tips.

[1] K. Kaiser et al., Science, 365, 1299-1301 (2019)
[2] L. Sun et al., Nature, 623, 972-976 (2023)
[3] Y. Gao et al. Nature, 623, 977-981 (2023)
[4] F. Albrecht et al. Science, 384, 677-682 (2024)

O 31.9 Tue 12:45 H24

**Temperature Induced Ring-Opening Polymerization Reaction for the Synthesis of Carbon Nanoribbons: Strain Influence on the On-surface Synthesis Using [6], [8]-, and [10]Cycloparaphenylenes** — •Miguel Wiche[1], Qigang Zhong[2], Daniel Kohrs[1], Qitang Fan[3], J. Michael Gottfried[4], Daniel Ebeling[1], Hermann A. Wegner[1], and André Schirmeisen[1] — [1]Justus Liebig University Giessen, Germany — [2]Soochow University, Suzhou, China — [3]University of Science and Technology of China, Hefei, China — [4]Philipps University Marburg, Germany

As the on-surface synthesis is an emerging reseach field, there is a lack of general understanding of reaction mechanisms, compared to conventional organic synthesis. Therefore, comprehensive research studies are required to figure out basic principles in the on-surface reaction mechanisms of organic molecules. In this work we investigate the strain influence of a set of Cycloparaphenylenes (CPP) in the temperature induced on-surface synthesis of biphenylene and graphene nanoribbons, using a strain induced ring opening polymerization (ROP) reaction. The decisive step of the polymerization, the ring opening, is found to strongly depend on the ring size and strain of the CPP molecules. Our work suggests that using smaller, highly strained rings, instead of rings with increasing number of phenyl units facilitates the ROP and nanoribbon formation.

# O 32: Heterogeneous Catalysis I

Time: Tuesday 10:30–12:45 Location: H25

O 32.1 Tue 10:30 H25

**Stability and reactivity of metal clusters on rutile $TiO_2$(110) under near-ambient pressure conditions** — •Marina Isabel de la Higuera Domingo, Florian Kraushofer, Matthias Krinninger, Friedrich Esch, and Barbara A. J. Lechner — Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, 85748 Garching, Germany

Clusters are widely recognized for their unique performance in heterogeneous catalysis as they exhibit discrete electronic states that lead to strongly size-dependent catalytic properties [1]. However, their application in industrial processes is often limited by their instability under reaction conditions. At elevated temperatures, clusters tend to sinter, which reduces their surface area and alters their catalytic behavior.

Reducible oxides, such as titania ($TiO_2$), are effective supports to stabilize clusters and tune their activity through encapsulation induced by the strong metal-support interaction (SMSI) [2]. While metal nanoparticles on $TiO_2$ are well-studied, much less is known about the dynamics of clusters, in particular at high temperatures and pressures. In the present work, we employ near-ambient pressure scanning tunneling microscopy (NAP-STM) to study the effect of reducing and oxidizing atmospheres on metal clusters on rutile $TiO_2$(110). We will also delve into the influence of the sample stoichiometry on its reactivity at different ambient conditions [3].

[1] A.Beck, et al. Nat.Commun. 2020, 3220.

[2] S.J. Tauster. Acc. Chem. Res. 1987, 389-394

[3] F. Kraushofer, et al. Nanoscale 2024, 17825-17837

O 32.2 Tue 10:45 H25

**Structural and chemical analysis of coexisting hexagoal and monoclinic phases of samarium oxide on Cu(111)** — •Björn Riedel, lars Buss, Raquel Sanchez-Barquilla, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany

The absence of in-depth spectroscopic and structural studies on model systems leads to a knowledge gap in understanding how the structure of samaria influences its chemical behavior. A multi-method approach has been employed to investigate the Cu(111)-supported $Sm_2O_3$ surface with high structural and chemical sensitivity by using low-energy electron microscopy (LEEM) in combination with X-ray absorption photoemission electron microscopy (XAS-PEEM) and other complementary methods such as micro-spot low-energy electron diffraction ($\mu$LEED) and X-ray photoelectron spectroscopy (XPS). Our measurements show the phase coexistence of small hexagonal A-$Sm_2O_3$(0001) islands and monoclinic B-$Sm_2O_3$(100) rectangular-shaped islands with different rotated rectangular domains. Furthermore, the redox properties of both $Sm_2O_3$ phases were studied by exposing the system to reducing ($H_2$) and oxidizing ($CO_2$) conditions, indicating a face-dependent reduction and oxidation behavior. Moreover, the monoclinic $Sm_2O_3$(100) islands appear less stable as they change to the hexagonal phase during annealing. These results indicate a highly dynamic system that can easily be adjusted by adapting the growth conditions, such as growth temperature and oxygen partial pressure.

O 32.3 Tue 11:00 H25

**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 often form key components of stable and well-performing industrial heterogeneous catalysts. Yet, today's industrial catalysts often only benefit from one or two promoters. This can often be traced back to the laborious empirical research required to identify promising formulations that jointly act to improve catalyst performance. To overcome such hurdles, we implemented an accelerated catalyst discovery approach by globally exploring a large catalyst design space using only a limited number of experiments. Its pillars are an efficient Design-of-Experiment (DoE) planning, a fast parallelized testing protocol and an iterative incorporation of experimental feedback. New and competitive promoter chemistries for the non-oxidative propane dehydrogenation to propylene over supported Pt were discovered in a limited experimental campaign. The results show the potential of iterative DoE strategies for the data-efficient knowledge-generation and optimization in complex, academically and industrially relevant catalytic systems.

O 32.4 Tue 11:15 H25

**Synergistic effect of oxygen and water on the environmental reactivity of 2D layered GeAs** — •Luca Persichetti[1], Giacomo Giorgi[2], Luca Lozzi[3], Maurizio Passacantando[3], Fabrice Bournel[4], Jean-Jacques Gallet[4], and Luca Camilli[1] — [1]University of Rome Tor Vergata, Italy — [2]University of Perugia, Italy; — [3]University of L'Aquila, Italy — [4]Sorbonne Université, CNRS, Paris, France

GeAs is a fascinating 2D material with compelling properties stemming from its intrinsic anisotropy. However, it reacts strongly with air, forming a Ge-oxide layer that affects its optoelectronic properties, such as contact resistance and refractive index. Investigating GeAs reactivity under realistic device conditions, including humid O2 and water exposure, is therefore crucial.

At the TEMPO beamline of Soleil, near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) was employed to study GeAs in the presence of oxygen and water. Results showed minimal reactivity with dry O2 and de-aerated water, while slight humidity (Rw = 0.5%, T = 20°C) in an O2 atmosphere significantly enhanced reactivity. Density functional theory calculations confirmed this synergistic effect, revealing a highly exothermic formation energy for the simultaneous chemisorption of O2 and H2O, compared to the adsorption of each molecule individually.

This research was supported by EU-funded MUR programs PRIN2022 ATYPICAL (2022JW8LHZ) and PRIN 2022-PNRR SPIGA (P2022LXNYN).

O 32.5 Tue 11:30 H25

**A comparative DFT+$U$ study of the oxygen evolution reaction at infinite-layer, brownmillerite and perovskite nickelates** — •Achim Füngerlings and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen, Duisburg, Germany

We present a detailed DFT+$U$ investigation of rare earth nickelates $R$NiO$_x$(001), $R$ = La, Nd; $x = 2, 2.5, 3$ as anode materials for the oxygen evolution reaction (OER). In these materials the Ni reaction sites at the surface exhibit different coordination, i.e. square-planar in the infinite layer ($x$ = 2, IL), fivefold coordination at the (001) perovskite surface ($x$ = 3) and both fourfold and fivefold coordination at the brownmillerite surface ($x$ = 2.5, BM). Voltammetry measurements find a lower onset potential for the catalytically much more active infinite layer compared to the perovskite counterparts.[1] Moreover, x-ray diffraction measurements suggest that the infinite layer gradually transform into brownmillerite during OER.[1] Our calculations confirm a lower overpotential for both the infinite layer and brownmillerite phases over the respective perovskite phase. The results reveal that the oxidation state of surface Ni has a more profound effect on the catalytic activity than the coordination number, with Ni$^{2+}$ (found at the IL and the fivefold coordinated BM site) leading to lower (0.53, 0.56 V for $R$=La; $x$=2, 2.5) and Ni$^{3+}$ (at the fourfold coordinated site in BM and the fivefold coordinated site at the perovskite surface) leading to higher overpotentials (0.67, 0.68 V for $R$=La; $x$=2.5, 3).

[1] M. Osada, A. Füngerlings, R. Pentcheva, and H. Y. Hwang, to be submitted.

O 32.6 Tue 11:45 H25

**How does lanthanum promote cobalt for ammonia synthesis in Co/$La_2O_3$ catalysts?** — •Clara C. Aletsee, Lau H. Wandall, Ke Zhang, Oliver Christensen, Jens K. Nørskov, and Ib Chorkendorff — Physics, Technical University of Denmark

The interest in developing catalysts for ammonia synthesis, operating under milder reaction conditions than the Haber-Bosch process, has increased in the last decades. Cobalt, typically unreactive, can be activated for ammonia synthesis through the addition of lanthanum in metallic or oxidized form.[1,2] To obtain a comprehensive understanding of the promotion mechanism, we investigate the ammonia formation over Co particles on $La_2O_3$ by combining experiments with theory. For this, we synthesized defined model catalyst, consisting of mass-selected Co nanoparticles, deposited on $La_2O_3$ films generated by magnetron sputtering. Their catalytic activity was tested at 1 bar and 350-500°C in a UHV-compatible reaction cell.[3] Catalyst states before and after reaction were analyzed by X-ray photoelectron spectroscopy and low-energy ion scattering. The results, combined with previous findings on the Co/LaN system,[2] suggest that the reaction proceeds on La-promoted Co steps due to spin-mediated effects supported by theoretical calculations.[4] We further demonstrate that the activity of the $Co/La_2O_3$ can be partially recovered after air exposure.

[1] S. I. Miyahara *et al.*, *ACS Omega* 7, 24452-24460 (2022). [2] K. Zhang *et al.*, *Science* 383, 1357-1363 (2024). [3] K. Zhang *et al.*, *Rev. Sci. Instrum.* 94, 114102 (2023). [4] A. Cao *et al.*, *Nat. Commun.* 13, 2382 (2022).

O 32.7 Tue 12:00 H25

**U-Ce charge transfer in epitaxial $Ce_{1-x}U_xO_2$ films grown on Ru(0001): consequences for thermochemical water splitting** — •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

Reducible metal oxides are crucial in applications like catalysis and solar energy conversion. Among these, cerium oxide ($CeO_2$) stands out for its stability and activity, yet its reduction requires high energy. Ceria doping or mixing with other elements has been proven successful in increasing the conversion from $Ce^{4+}$ to $Ce^{3+}$. Uranium cations are the most suitable candidates: 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. The fundamental study of the charge transfer process requires model systems, as heat and mass transfer limitations are largely absent compared to polycrystalline powders. By in-situ X-ray photoelectron spectroscopy (XPS) and low-energy electron diffraction (LEED), we explored the redox properties and structural stability of epitaxial (111)-oriented $Ce_{1-x}U_xO_2$ on Ru(0001). The as-grown films, prepared by reactive direct current sputtering from metallic targets, show a high $Ce^{4+}$ to $Ce^{3+}$ conversion, reversible upon reducing-oxidizing cycles. The experimental results are discussed in the light of density function theory (DFT) calculations.

O 32.8 Tue 12:15 H25

**Accelerating Surface Adsorption Energy Prediction with Machine Learning Foundation Models** — •Karlo Sovic[1,2] and Johannes T. Margraf[2] — [1]University of Zagreb Faculty of Science — [2]University of Bayreuth

Determining the adsorption energies of molecular adsorbates on surfaces is critically important in heterogeneous catalysis, as well as in many other fields of materials science and chemistry. Understanding the nature and strength of adsorbate-surface interaction leads to a more rational design of efficient catalysts and improvements in their performance. While accurate first-principles calculations have brought about a revolutionary advance in our ability to predict properties and design materials *in silico*, high computational costs and poor scaling limit their application in exploring complex real-world materials. Machine-learning interatomic potentials offer a solution to this materials exploration problem. In particular, the recent emergence of pre-trained foundation models offers a data-efficient route to obtain accurate models via fine-tuning. To showcase their efficiency and performance, extensive computational research has been conducted using a fine-tuned MACE-MP-0 model to study the adsorption of glycerol on various metallic surfaces in the gas phase. This talk will present the methodology for investigating the global minima of complex adsorbate molecules on various metal surfaces, determining their respective adsorption energies, and exploring various reaction mechanisms on adsorbent's surface through computational approaches.

O 32.9 Tue 12:30 H25

**Role of Co-Catalyst Loading in the Photoreforming of Tertiary Alcohols at Ambient Pressure on Titania P25** — •Paula Neumann, Clara Aletsee, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Efficient semiconductor photocatalysts are usually modified with a so-called co-catalyst, a metal particle which is commonly assumed to promote charge separation, but whose exact role remains elusive. To elucidate the influence of platinum particles loaded onto a titania powder catalyst we investigated the photoconversion of tertiary alcohols in our gas phase-photoreactor at ambient conditions. Different to its usual interpretation but in accordance with UHV studies we show that the co-catalyst facilitates the recombination of surface hydrogen. Thereby, a second reaction pathway is opened up where a C-C coupling product forms on the titania surface. Hence, identifying the mechanistics of alcohol photochemistry is not only providing insights into hydrogen formation but it also sheds light onto complex alkyl coupling reactions.

## O 33: Poster Graphene: Electronic Structure and Excitations

Time: Tuesday 13:30–15:30 Location: P3

O 33.1 Tue 13:30 P3

**Reversible transition between $(10 \times 10)$ and $(11 \times 11)$ phases of Pb intercalated EG on 6H/SiC(0001)** — •Sergii Sologub[1,2], Markus Gruschwitz[2], Bharti Matta[3], Andres David Pena Unigarro[2], Philipp Rosenzweig[3], Sibylle Gemming[2], Kathrin Küster[3], Ulrich Starke[3], and Christoph Tegenkamp[2] — [1]Institute of Physics, NAS of Ukraine, Kyiv — [2]Institut für Physik, TU Chemnitz, Chemnitz — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart

Epitaxial graphene (EG) obtained by intercalation of a buffer layer on 6H/SiC(0001) with Pb atoms is the subject of intensive experimental and theoretical studies due to its charge neutrality, the band gap opening and proximity superconductivity. The hallmark of Pb-intercalated EG is the formation of diffraction spots with $(10 \times 10)$ or $(11 \times 11)$ periodicity in the high-resolution LEED patterns. The correlation between these phases and corresponding microstructure, i.e. “striped” and “bubble” Pb intercalated phases, were examined by STM and by dark field imaging in a photoemission electron microscope. We have also established a recipe to reversibly switch between the $(10 \times 10)$ and $(11 \times 11)$ structures. In addition, the ratio of areas occupied by these coexisting phases could be estimated from the intensity ratio of second order LEED spots. Importantly, the degree and ease of intercalation strongly depends on the defect density of the initial buffer layer. The transformation between the different phases can be rationalized by the low diffusion barrier of Pb on SiC observed by density functional calculations.

O 33.2 Tue 13:30 P3

**Confinement-mediated intercalation of metals in epitaxial graphene: Unlocking room temperature intercalation** — •Kathrin Küster[1], Stefan Wundrack[2,3], Markus Gruschwitz[4], Sawani Datta[1], Bharti Matta[1], Teresa Tschirner[2], Marius Eckert[2,3], Rainer Stosch[2], Christoph Tegenkamp[4], Ulrich Starke[1], Klaus Pierz[2], and Andrey Bakin[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Physikalisch-Technische Bundesanstalt, Braunschweig — [3]Institut für Halbleitertechnik - TU-Braunschweig — [4]Institut für Physik, TU Chemnitz

Intercalation of materials underneath epitaxial graphene is an effective way to tune graphene's properties but also to stabilize otherwise unstable 2D materials. Usually, this procedure requires extreme conditions like ultra-high vacuum and elevated temperatures often above 400 °C. Within the DFG research unit FOR 5242 we also investigate alternative routes of intercalation under more accessible conditions. Here, we report on the intercalation of Ga and In under monolayer graphene at ambient conditions. A multi-technique approach combining spectromicroscopy techniques with density functional theory calculations gives detailed insights into the intercalation pathways and the diffusion of the intercalants at the interface between graphene and the SiC substrate. It is evident that the intercalated atoms are strongly bound to the topography of the SiC terraces during their diffusion and exhibit anomalies in their diffusion behavior. The monolayer graphene is transformed into a decoupled bilayer upon intercalation and the intercalated materials develop their own metallic 2D electronic structure.

O 33.3 Tue 13:30 P3

**Proximity-effects in epitaxial graphene: recent highlights of our Research Unit FOR5242** — S. Gemming[1], I. Gierz-Pehla[2], K. Küster[3], K. Pierz[4], Th. Seyller[1], U. Starke[3], •C. Tegenkamp[1], T. Wehling[5], and M. Wenderoth[6] — [1]Institut für Physik, TU Chemnitz — [2]Institut für Experimentelle und Angewandte Physik, U Regensburg — [3]Institut für Festkörperforschung, MPI Stuttgart — [4]Physikalisch-Technische Bundesanstalt, Braunschweig — [5]Institut für Theoretische Physik, U Hamburg — [6]IV. Physikalische Institut, U Göttingen

Proximity effects in low dimensional electron gases are essential for the design of new quantum materials with tailored electronic, magnetic and optical properties. A recent example is superconductivity in twisted bilayer graphene. Our Research Unit FOR 5242 studies the influence of proximity-induced spin-orbit interaction (SOI), electronic correlations as well as local electric fields on 2D electron gases, using epitaxial graphene (EG) on SiC substrates as a model system. EG is known for its flexible functionalization schemes including intercalation and adsorption, enabling control of the doping level, hybridization effects, and the strength of the Coulomb interaction. Here, we highlight a few of our recent results including (1) the use of EG for quantum Hall resistance standards, (2) SOI in graphene induced by 2D Pb layers, (3) Mott-Hubbard physics realized by the intercalation of Sn and Si, (4) many-body effects in extremely doped EG and (5) novel 2D interface layers. For further details see www.for5242.de

O 33.4 Tue 13:30 P3

**Quasi-freestanding monolayer graphene achieved by Pb intercalation** — •S Wolff[1], P Schädlich[1], A D Peña Unigarro[1], B Matta[2], G Ghosal[1], F Schölzel[1], P Richter[1], M Hutter[3], M Stettner[3], K Küster[2], C Kumpf[3], S Gemming[1], U Starke[2], C Tegenkamp[1], and T Seyller[1] — [1]Institute of Physics, TU Chemnitz — [2]MPI für Festkörperforschung, Stuttgart — [3]Peter Grünberg Institut, Forschungszentrum Jülich

Intercalation is a promising approach for tailoring the electronic structure of epitaxial graphene on SiC. Beyond that, it enables the formation of otherwise unstable 2D phases of elements and opens a route to study the interplay between the two 2D materials and the substrate. We have studied the Pb intercalation process under the buffer layer in detail using low-energy electron microscopy (LEEM), photoelectron spectroscopy (PES), scanning tunneling microscopy (STM), density functional theory calculations (DFT) and X-ray standing wave (XSW). LEEM is used to monitor the intercalation process at different intercalation temperatures, resulting in either a $(1 \times 1)$ symmetry or in a $(10 \times 10)$ superstructure of the Pb atoms. These findings can be supported by angle-resolved PES and STM. Experiments indicate, in agreement with DFT, different filling of the Pb bands depending on the SiC polytype. Furthermore, XSW was used to determine the interlayer distances, revealing covalent bonding of the intercalant to the substrate and van der Waals bonding to graphene.

O 33.5 Tue 13:30 P3

**Liquid metal intercalation of epitaxial graphene Hall bar devices on SiC** — •Marc Bothe[1,2], Stefan Wundrack[1,2], Teresa Tschirner[1], Markus Gruschwitz[3], Yefei Yin[1], Klaus Pierz[1], Frank Hohls[1], Rainer Stosch[1], Christoph Tegenkamp[3], Hans Werner Schumacher[1], and Andrey Bakin[2] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Institut für Halbleitertechnik, TU Braunschweig, Hans-Sommer-Str. 66, 38106 Braunschweig — [3]Institut für Physik, Technische Universität Chemnitz, Reichenhainer Strasse 70, 09126 Chemnitz, Germany

Epitaxial graphene grown on SiC is a promising platform for metal intercalation, enabling the investigation of proximity effects. Metal intercalation relies on the controlled introduction of lattice defect densities in monolayer graphene, achieved through plasma treatment. This is followed by liquid metal intercalation, during which atoms diffuse through lattice defects and propagate beneath the graphene. However, the use of metal intercalated graphene samples for device fabrication presents two challenges. First, solvents used for lithography often lead to metal deintercalation. Second, lattice defects in graphene compromise the structural and electronic integrity of the graphene device. We use an alternative strategy that combines lithography with metal intercalation through predefined channels. Initial measurements of Hall bar structures intercalated with gallium show superconducting behavior, demonstrating the potential of this approach for advanced device applications.

O 33.6 Tue 13:30 P3

**Mesoscopic Lateral Intercalation Dynamics of Tin Between the Epitaxial Buffer Layer of Graphene and SiC** — •Benno Harling[1], Zamin Mamiyev[2], Christoph Tegenkamp[2], and Martin Wenderoth[1] — [1]IV. Physical Institute, Georg-August-University Göttingen, Germany — [2]Analysis of Solid Surfaces, Nanostructures and Quantum Materials, TU Chemnitz, Germany

Within the challenges of modern electronics, the dynamics of intercalation in layered structures is key for pushing the boundaries of technological limits. Fine-tuned control and a deeper understanding of the intercalation process is needed. Our study focuses on the lateral dynamics of this intercalation process. Whereas penetration of the graphene sheet was already often discussed [1], the lateral atom transport processes according to the mesoscopic landscape of the substrate has been less addressed. Kelvin Probe Force Microscopy (KPFM) was used to investigate an epitaxial graphene buffer layer intercalated with tin. A diffusion edge to the pristine buffer layer can be identified with this method down to the mesoscopic scale below 100 nanometers. On a vicinal surface, we find surface steps as a clear barrier for diffusion. Material transfer over the substrate steps is mediated by a local defect, i.e. local pin-holes. Moreover, we do not observe nucleation on the terrace, but the decoration of the next step by tin. Faster diffusion at the step edges leads to directional growth of the intercalated phase.

Financial support by the DFG within research unit FOR5242 is greatly acknowledged.

[1] Wu et al., Prog. Surf. Sci. 96, 100637, 2021

O 33.7 Tue 13:30 P3

**Magnetic MnPc molecules adsorbed on epitaxial graphene** — •James Oyuga[1], Nhung Nguyen[1], Uwe Gerstmann[2], Eva Rauls[3], Julian Koch[1], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Germany — [2]Theoretische Physik, Universität Paderborn, Germany — [3]Department of Mathematics and Physics, University of Stavanger, Norway

Phthalocyanines (Pc) are prototype molecules hosting magnetic ions. When adsorbed on surfaces, the spin state of the molecules is influenced by the substrate. In a combined experimental and theoretical study, we investigated this influence for the case of MnPc molecules adsorbed on monolayer graphene/SiC(0001) using STM, magnetotransport and theoretical DFT modeling. The STM measurements showed that the self-assembly of the MnPc molecules results in an almost defect-free monolayer with a $(4 \times 2)$ unit cell accommodating 8 MnPc molecules. The DFT modeling revealed that the structure and thereby the spin states of the molecules are decisively influenced by the substrate. In the gas phase the MnPc molecules are symmetrically bended with a spin state of $S = 3/2$. However, on an epitaxial graphene monolayer this is changed into an even mixture of flat molecules with an $S = 5/2$ spin state and upward bended molecules with an $S = 3/2$ spin state. This mixture allows for a denser arrangement of the molecules in a $(4 \times 2)$ unit cell, that is commensurable with both the graphene layer and the underlying SiC substrate. The impact of such molecular structures towards transport in epitaxial monolayer graphene is quantified by magneto transport experiments analyzing the weak (anti) localization.

O 33.8 Tue 13:30 P3

**Intercalation of a condensed 2D-Ag phase within the epitaxial graphene/SiC interface** — •Sawani Datta[1], Vibha Reddy[1], Bharti Matta[1], Arpit Jain[2], Kathrin Küster[1], Joshua A. Robinson[2] und Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Pennsylvania State University, State College, USA

Intercalating 2D materials at the epitaxial graphene (EG)/SiC interface improves their environmental stability, facilitating the use of various ex-situ techniques for their fundamental study and application purposes. In a previous study, we showed that Ag atoms intercalated at the EG/SiC interface form a triangular $(1\times1)$ lattice with respect to the SiC and the Ag interlayer is semiconducting [1,2]. Interestingly, intercalating Pb into a previously Ag-intercalated sample results in the complete replacement of Ag by Pb. Subsequently, another round of Ag intercalation can entirely replace Pb, forming a new Ag phase characterized by a 4/3 packing of Ag with respect to the underlying

Si layer. Theory suggested the existence of two intercalated 2D material phases also for several other materials [3] and Auger electron spectroscopy mapping indeed shows a higher Ag concentration of the latter Ag phase [4]. In this work, we compare the 2 different Ag phases by low-energy electron diffraction (LEED) and angle-resolved photoemission spectroscopy (ARPES). This ongoing study is supported by DFG through FOR 5242 and by NSF Grant DMR-2011839. [1] Phys. Rev. B 101, 201407(R) (2020). [2] Phys. Rev. B 105, 235428 (2022). [3] arXiv:2011.01914v1 (2020). [4] 2D Materials 8, 41003 (2021).

O 33.9 Tue 13:30 P3

**Scanning tunneling potentiometry methods for intercalated graphene systems** — •Tim Güldenpfennig[1], Simeon Bode[2], Markus Gruschwitz[1], Martin Wenderoth[2], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Germany — [2]IV. Physikalisches Institut, Universität Göttingen, Germany

Graphene and graphene-based (hetero-)systems were subjects in a wide range of studies in the past decades revealing their intriguing electronic properties. Epitaxially grown graphene on SiC plays a vital role as a base for electronic application. By intercalating such grown buffer layer with different elements the electronic properties of the decoupled graphene layer can be precisely manipulated. Recently a great interest in the two dimensional intercalant layers arose as well. The latest advance towards intercalation of heavy elements (Pb, Bi, etc.) comes along with new challenges due to defect-dependent intercalation paths. Macro- and mesoscopic transport experiments on these percolated but multi-scale defective intercalated phases become impractical [1].

For transport investigations at the nanometer scale we utilize scanning tunneling potentiometry (STP). In combination with finite element simulations the conductivity of the intercalated phase and the influence of defects can be separated precisely. Two different setups to investigate the transport properties of intercalated graphene systems on nanoscopic scale are presented. One is implemented in a 4pp-STM/SEM setup with the ability to locally apply transverse voltages. The other setup uses an home-built STM for measurements at 6 K with micro-Volt resolution. [1] Phys. Rev. B 109, 245430 (2024)

O 33.10 Tue 13:30 P3

**Electronic and structural properties of a Sn Mott phase proximitized to graphene** — C. Ghosal[1], •H.-T. Ngo[1], S. Ryee[2], Z. Mamiyev[1], N. Witt[2,3], T. Wehling[2,3], and C. Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz — [2]Institute of Theoretical Physics, U Hamburg — [3]The Hamburg Centre for Ultrafast Imaging, Hamburg

Graphene, renowned for its exceptional electronic and optical properties as a robust 2D material, traditionally lacks electronic correlation effects. Proximity coupling offers a promising method to endow quantum materials with novel properties. In this study, we achieved such a proximity coupling by intercalating Sn between the buffer layer of graphene on SiC(0001). In the $\sqrt{3}$-areas, the Sn-$p_z$ electrons exhibit robust correlation effects manifest as characteristic Hubbard bands analyzed by STS and EELS. Thereby, the system revealed a spatially modulated hybridization between the Dirac and the correlated electrons depending on the Sn sites with respect to the graphene lattice. The DFT and DMFT calculations show excellent agreement regarding the spectral properties. The analyses revealed further that besides the hybridization and Coulomb interaction also the charge transfer plays an important role for electronic state that emerges in these artificial correlated systems.

O 33.11 Tue 13:30 P3

**Twisted Bilayer Graphene by Hydrogen Intercalation** — •Hao Yin[1,2], Andrei Matetskii[1], Frank Stefan Tautz[1,2], François C. Bocquet[1], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), FZ-Jülich, Germany — [2]RWTH Aachen University, Aachen, Germany

Quasi-free-standing twisted bilayer graphene (TBLG) with a 30° twist angle is achieved on a 6H-SiC(0001) surface via hydrogen intercalation of the zeroth-layer graphene (ZLG). Initially, 0°-rotated monolayer graphene is prepared using the surfactant-mediated epitaxial growth method [PRL **125**, 106102 (2020)]. The processes of hydrogen intercalation and deintercalation were investigated using Low Energy Electron Microscopy (LEEM), with intercalation conducted stepwise, while deintercalation was monitored in real time. Our results provide valuable insights into the mechanisms underlying hydrogen intercalation and deintercalation.

A sharp reaction front was observed, aligned parallel to the step edges, suggesting that hydrogen atoms migrate beneath the ZLG from surface discontinuities, such as step edges or defects.

Deintercalation, taking place 200°C above the intercalation temperature, was significantly faster (within one minute) and occurred uniformly, as indicated by the homogeneous brightness changes in deintercalated regions. This implies a much faster diffusion of H under the TBLG at this temperature, or possibly that H atoms are able to penetrate through the graphene layers.

O 33.12 Tue 13:30 P3

**Near-Field Optical spectroscopy of few-layer Graphene's interband resonances to study it's gate-tunable band structures** — •Dominique Malik, Lina Jäckering, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

The band structure of few-layer graphene (FLG) defined by the crystallographic stacking order determines its electronic and optical properties. Optical spectroscopy of interband resonances - the excitation of electron transitions between two electronic bands - allows to directly probe the gate-tunable band structure. Within one flake FLG can exist in different stacking orders. However, conventional far-field spectroscopy is diffraction limited and cannot resolve stacking domains below this limit [1]. Recently, with scanning near-field optical microscopy (s-SNOM) the interband resonances of bilayer graphene (BLG) and 4LG have been retrieved [2]. Due to the stacking specific resonance energy, s-SNOM spectroscopy allowed for the identification of stacking domains on the nanometer scale [2]. The local effect of the application of a gate voltage to FLG has not been studied. Here, we present the theoretical foundation to perform near-field optical spectroscopy of interband resonances of gated trilayer and BLG over the energy range from 0.28 to 0.54 $eV$ to gain insights into gate-tunable modifications of their band structures. We layout the design and fabrication of a suitable sample and show initial results. We expect high-resolution s-SNOM measurements could reveal local variations in band gap opening, which are unachievable with far-field techniques. [1] Lui et al. Nano Lett. 11, 1 (2011) [2] Wirth et al. ACS Photonics 8.2 (2021)

O 33.13 Tue 13:30 P3

**non-equilibrium carrier dynamics of a graphene - 2D Mott insulator interface** — Maria-Elisabeth Federl[1], •Franziska Bergmeier[1], Zamin Mamiyev[2], Niklas Witt[3], Tim Wehling[3], Christoph Tegenkamp[2], and Isabella Gierz[1] — [1]University of Regensburg — [2]Technical University Chemnitz — [3]University of Hamburg

Hybridization between localized and itinerant electrons is believed to be responsible for the formation of exotic electronic states including heavy-fermion behaviour or unconventional superconductivity. Confinement heteroepitaxy, where novel 2D structures are stabilized at the interface between epitaxial graphene and SiC substrate, provides a pathway to engineer proximity-coupling between the massless carriers in graphene and the carriers in the underlying layer. We intercalated graphene with Sn, where the ($\sqrt{3} \times \sqrt{3}$)R30° phase formed on SiC(0001) is believed to be a Mott insulator [1], and used time- and angle-resolved photoemission spectroscopy (trARPES) as well as density functional theory (DFT) to search for indications of interlayer hybridization that might pave the wave towards the realization of exotic electronic phases.

[1] Phys. Rev. Lett. 114, 247602 (2015)

O 33.14 Tue 13:30 P3

**Sequential Intercalation of Epitaxial Graphene with Multiple Elements** — •Niels Rösch, Mohammad Elkhawaga, Philip Schädlich, Fabian Göhler, and Thomas Seyller — Chemnitz University of Technology, Institute of Physics, 09126 Chemnitz, Germany

The intercalation of epitaxial graphene on SiC(0001) is a field of research that currently attracts attention. On one hand it provides the possibility to fine-tune the properties of the graphene layer. On the other hand it also is a means to fabricate two-dimensional materials in a confined state [1,2].

In this study we test the possibility to synthesize binary compounds by sequential intercalation of two elements. As test cases we have chosen the topological insulator $Bi_2Se_3$ [3] and the superconductor FeSe [4]. To that end, Bi or Fe is first intercalated using a deposition and annealing approach. This is followed by an exposure to a selenium-rich atmosphere at elevated temperatures. Samples are characterized by photoelectron spectroscopy and electron diffraction.
[1] Z. Y. Al Balushi et al., Nat. Mater (2016) 1166.

[2] N. Briggs et al., Nat. Mater. 19 (2020) 637.
[3] H. Zhang et al., Nat. Phys. 5 (2009) 438.
[4] J.-F. Ge et al., Nat. Mater. 14 (2014) 285.

O 33.15 Tue 13:30 P3

**Free-standing graphene films/membranes** — •Leon Lasnig, Lukas Kalkhoff, Steffen Franzka, and Marika Schleberger — Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany

Large-area graphene films are usually grown onto a copper sheet via chemical vapor deposition. The transfer of the graphene to another substrate to this date has been done with the help of polymer films, which leads to impurities and residues. These residues can change the properties of graphene. It is therefore necessary to develop new fabrication protocols to prevent or at least minimize contaminations.
Here we present a new technique for fabricating membranes without the requirement of an PMMA layer. The samples were then transferred on hole substrates with a hole diameter of $150\,\mu$m. Since a monolayer is not stable enough to cover the hole, samples with multiple layers were prepared. These were characterized using Raman spectroscopy and an optical profilometer. Raman spectroscopy showed that the samples within the holes are very homogeneous in terms of doping and strain. The lack of D mode in the measured Raman spectra indicates a clean sample. The profilometer revealed that the graphene membranes in the holes have an average hight deviation of only 138 nm.

O 33.16 Tue 13:30 P3

**Electronic and structural properties of Bi-intercalated epitaxial graphene on SiC(0001)** — Niclas Tilgner[1], Susanne Wolff[1], Andres D. Peña Unigarro[1], Philip Schädlich[1], Fabian Göhler[1], Bharti Matta[2], Philipp Rosenzweig[3], Kathrin Küster[2], Mark Hutter[4], Monja Stettner[4], Hao Yin[4], Serguei Soubatch[4], François C. Bocquet[4], Tien-Lin Lee[5], Christian Kumpf[4], Ulrich Starke[2], Sibylle Gemming[1], and •Thomas Seyller[1] — [1]Institut für Physik, TU Chemnitz — [2]Max Planck Institut für Festkörperforschung, Stuttgart — [3]Physikalisches Institut, Universität Stuttgart — [4]Peter Grünberg Institut, Forschungszentrum Jülich — [5]Diamond Light Source, United Kingdom

The intercalation of epitaxial graphene on SiC(0001) is a research area that currently attracts attention. Not only does it provide the possibility to fine-tune the properties of the graphene layer, it also allows fabricating two-dimensional materials in a confined state. Using a variety of experimental (LEED, LEEM, XPS, ARPES, XSW) and theoretical (DFT) approaches we studied the structural and electronic properties of different intercalated Bi phases that are formed depending on the preparation conditions. While a dense phase with a $(1\times1)$ periodicity with respect to SiC(0001) shows metallic properties, a diluted $(\sqrt{3}\times\sqrt{3})R30^\circ$ phase appears insulating. Upon annealing in hydrogen, the latter can be transformed into a layer of bismuthene. However, while the bismuthene is arranged with the same periodicity, DFT calculations suggest that the transition is accompanied by a major structural rearrangement.

O 33.17 Tue 13:30 P3

**Transport Properties of Epitaxial Graphene on 4H-SiC(0001) and 6H-SiC(0001) on the Local Scale** — •Simeon Bode[1], Benno Harling[1], Teresa Tschirner[2], Klaus Pierz[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig

Recent experiments on epitaxial graphene on silicon carbide have shown that transport properties strongly depend on the surface termination of the SiC substrate. Here, we study the impact of the polytype of the substrate SiC on various local properties of Polymer Assisted Sublimation Grown (PASG) graphene. Recently, it has been shown that there are two different surface terminations present at 6H-SiC [1], whereas mainly one surface termination was observed on 4H-SiC. The structural properties are investigated by STM and AFM, whereas electronic properties are extracted from STS data. Local transport measurements using Scanning Tunneling Potentiometry (STP) on 6H-SiC reveal variations in the sheet resistance from terrace to terrace when changing the stacking sequence across a step. On the other hand, the local sheet resistances of neighbouring terraces are very similar if the step height is half of a SiC unit cell, i.e., having the same termination on both sides. PASG graphene on 4H-SiC predominantly exhibits steps of half the unit cell. First data on 4H-SiC indicates that also on this system the sheet resistance is only slightly varying across steps. This work was financially supported by the DFG through the FOR5242. [1] Sinterhauf et al., Nat Commun 11, 555, 2020

O 33.18 Tue 13:30 P3

**Growth dynamics of the graphene buffer layer on SiC(0001) grown by polymer-assisted sublimation growth (PASG)** — •Julia Guse[1], Teresa Tschirner[1], Stefan Wundrack[1], Kathrin Küster[2], Ulrich Starke[2], Philip Schädlich[3], Thomas Seyller[3], Klaus Pierz[1], and Hans Werner Schumacher[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart — [3]Institut für Physik, TU Chemnitz

Fabrication of two-dimensional (2D) heterostructures using epitaxial graphene on SiC is gaining interest for engineering new electronic material systems. Important for the quality of the epigraphene layer is the 0th graphene layer, the buffer layer, being covalently bonded to the SiC substrate. However, there is still conflicting theoretical and experimental evidence of the structural properties of the buffer layer and its influence on epigraphene. Further, the quality of this buffer layer is not well defined and systematic studies are still lacking. We use an advanced growth technique preventing step bunching and large terrace step heights to achieve high quality buffer layer on millimeter scale. The buffer layer is grown by thermal sublimation in an argon atmosphere and by applying the polymer-assisted sublimation growth (PASG) method. By pretreatment of the SiC substrate which supplies additional carbon during the initial nucleation process the SiC surface is stabilized by rapid buffer layer formation which prevents step bunching. We investigate the growth parameters for homogeneous buffer layer formation and systematically study its growth dynamics.

O 33.19 Tue 13:30 P3

**Modeling the intercalation of epitaxial graphene with main group elements from first-principles** — Andres D. Peña Unigarro[1], Niklas Witt[2,3], Maria-Elisabeth Federl[4], •Alexander Korn[1], Isabella Gierz[4], Tim Wehling[2], Florian S. Günther[5], and Sibylle Gemming[1,6] — [1]Inst. Physik, TU Chemnitz — [2]Inst. Theoretische Physik, U Hamburg — [3]Theoretische Physik, JMU Würzburg — [4]Inst. Experimentelle und Angewandte Physik, U Regensburg — [5]UNESP, Rio Claro, Brazil — [6]MAIN Center, TU Chemnitz.

Intercalation of epitaxial graphene on silicon carbide (EG) with metallic interlayers opens up a plethora of fascinating physical phenomena, rooted in both spatial confinement and proximity coupling effects. A rich variety of exotic electronic states is obtained by the simultaneous presence of flat and Dirac-like bands with intricate splittings of the spins and pseudospins in EG and the intercalant.

Here, we present first-principles calculations for supercell models, which capture the essential structural and electronic properties of thin intercalation layers in EG. Ordered structures with different interlayer coverages have been studied, which provide distinctly tailored degrees of proximity coupling. Comparing interlayers from the experimentally well-studied main group elements Sn, Pb, and Bi allows distinguishing between isovalent and heterovalent intercalants as well as studying the influence of relativistic effects, in particular spin-orbit coupling (https://www.epigraphene.de/).

O 33.20 Tue 13:30 P3

**Influence of doping on non-equilibrium carrier dynamics in graphene** — •Leonard Weigl[1], Johannes Gradl[1], Peter Richter[2], Thomas Seyller[2], Camilla Coletti[3], and Isabella Gierz[1] — [1]University of Regensburg, Germany — [2]Technical University of Chemnitz, Germany — [3]Instituto Italiano di Tecnologia, Pisa, Italy

The understanding of non-equilibrium charge carrier dynamics in the quasi-relativistic dispersion of graphene is a key ingredient for the design of future ultrafast electronic devices. Despite its crucial importance for device operation, the role of the doping level remains controversial. Here, we use time- and angle-resolved photoemission spectroscopy (tr-ARPES) to study the energy-resolved photo-carrier relaxation in epitaxial graphene for different doping levels. In contrast to previous studies on the same material [1], we find the energy-resolved relaxation times to be independent of doping. We attribute this to the fact that - with increasing doping level - the peak electronic temperature is found to decrease, making the phase space for carrier relaxation doping-independent. Therefore, we speculate that the previously observed differences in carrier dynamics between graphene resting on C-and H-terminated SiC substrates, respectively, originate from the different interfaces to the substrate rather than the doping level. [1] J. C. Johannsen et al., Nano Lett. 15, 326-331 (2014)

O 33.21 Tue 13:30 P3

**Hexagons on Rectangles: Epitaxial Graphene on Ru$(10\bar{1}0)$** — •Lars Buss[1], Giovanni Zamborlini[2], Cathy Sulaiman[1], Moritz Ewert[1], Mirko Cinchetti[2], Jens Falta[3], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Germany — [2]Department of Physics, TU Dortmund University, Germany — [3]Institute of Solid State Physics, University of Bremen, Germany

The miniaturization of integrated electronics drives the demand for barrierless interconnects, with graphene-ruthenium structures emerging as promising candidates. We present an *in situ* study of the growth and electronic properties of graphene on rectangular Ru$(10\bar{1}0)$ grown by high-temperature carbon segregation. Using low-energy electron microscopy (LEEM), it is shown that graphene grows preferentially along the $[1\bar{2}10]$ direction, forming micrometer-sized rectangular islands. Microspot low-energy electron diffraction ($\mu$LEED) reveals two predominant graphene orientations, rotated by 0° (R0) and 30° (R30), with indications for the formation of graphene nanoribbons in bilayer graphene/Ru$(10\bar{1}0)$. Microspot angle-resolved photoemission spectroscopy ($\mu$ARPES) shows that the Dirac cones remain intact in bilayer graphene with reduced n-type doping compared to graphene/Ru(0001), indicating a weaker interaction with the Ru$(10\bar{1}0)$ surface. These results highlight the influence of substrate symmetry and interactions on graphene properties and provide insights for engineering graphene beyond hexagonal substrates.

## O 34: Poster Solid-Liquid Interfaces: Reactions and Electrochemistry

Time: Tuesday 13:30–15:30 Location: P3

O 34.1 Tue 13:30 P3

**Free Energy Calculations of Electrolyte Decomposition Reactions on Lithium Battery Electrodes** — •Azad Kirsan and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg

For the development of lithium metal batteries (LMBs) it is essential to understand how a stable solid electrolyte interphase (SEI) is formed. Ethylene carbonate (EC), a commonly used electrolyte, plays a critical role in SEI formation through its electrochemical decomposition at the electrode surface. Thus, insights into the mechanism of the decomposition reaction are of crucial importance for understanding the processes that govern SEI composition, structure and stability.

In this work, *ab initio* molecular dynamics simulations using state-of-the-art enhanced sampling methods (metadynamics, umbrella sampling, well-sliced metadynamics [1]) including explicitly the liquid electrolyte were performed in order to unravel the reaction mechanisms of the first steps of the EC dissociation on a $Li_2O$ surface. The trajectories, encompassing more than 1 ns of sampling time, were used to reconstruct the free energy surfaces and obtain activation barriers for the decomposition reaction.

[1] S. Awasthi, V. Kapil, N.N. Nair, J. Comput. Chem. **37** (2016) 1413

O 34.2 Tue 13:30 P3

**Optimizing Parameters in Metadynamics Simulations for Free Energy Calculations** — •Marlene Sell, Azad Kirsan, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg

The calculation of free energy surfaces (FES) is essential for understanding chemical reactions. Especially the free energy differences between educts, products and possible transition states, as well as the structure of the latter, allow insight into the nature of the reactions. Well-sliced metadynamics (WS-MTD) [1] is a novel method to calculate FES. It combines umbrella sampling and metadynamics in order to speed up the simulations. However, it employs several fine-tuning parameters whose exact influence on the efficiency and accuracy of the results is not yet well understood.

In this study, the FES of the reaction of 1,3-butadiene and ethylene to cyclohexene, the simplest Diels-Alder reaction, was calculated by WS-MTD. This reaction is well studied, both experimentally and theoretically, and could thus be used to compare the influence of the studied parameters. Using FES calculated with different values of the relevant parameters, the free energy differences between the educts, transition state and products were determined in the form of the activation barrier and reaction energy. These were compared to literature values from experimental and other theoretical studies.

[1] S. Awasthi, V. Kapil, N.N. Nair, J. Comput. Chem. **37** (2016) 1413

O 34.3 Tue 13:30 P3

**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

Detailed insights into solid-liquid interfaces are crucial for understanding many processes in catalysis and electrochemistry. Accurately modeling these interfaces using first-principles methods is computationally very demanding, which strongly restricts the complexity of the systems that can be studied. Machine learning potentials now can provide an efficient alternative with almost no loss in accuracy. In this study, high-dimensional neural network potentials (HDNNPs) are employed to investigate the Pt(111)-water interface in detail. After training to DFT reference data, molecular dynamics simulations are utilized to uncover the structural and dynamical properties of the interfacial water molecules.

O 34.4 Tue 13:30 P3

**Studying Tricalcium Silicate-Water Interfaces Using High-Dimensional Neural Network Potentials** — •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 advent of machine learning potentials (MLP) trained to 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 numerous solid minerals. In this study, we investigate interfaces of liquid water with alite ($Ca_3SiO_5$), an important cement mineral exhibiting various polymorphic states. Using large-scale MD simulations, an analysis of the structural and dynamical properties of interfacial water is presented.

O 34.5 Tue 13:30 P3

**Electrocatalytic $CO_2$ Reduction in Ionic Liquid/Nitrile Electrolytes** — •Björn Ratschmeier, Arik Geringswald, Alisa Kamaric, and Björn Braunschweig — University Münster, Institute of Physical Chemistry, Münster, Germany

Room-temperature ionic liquids (RTILs) play an important role in $CO_2$ reduction reactions ($CO_2$RR), providing a viable alternative to aqueous electrolytes, but face challenges such as high overpotentials and product selectivity. As we have previously shown for 1-butyl-3-methylimidazolium trifluorosulfonylimide ([BMIM][$NTf_2$]) electrolytes [1], the accessibility of water as a co-reactant at the interface is a limiting factor for CO formation potentials. To modulate the interfacial structure, different concentrations of acetonitrile and benzonitrile were introduced into [BMIM][$NTf_2$] electrolytes in the presence of 1.5 M $H_2O$. The resulting mixtures were investigated in terms of $CO_2$RR at polycrystalline Au electrodes. The presence of 7.5 M benzonitrile resulted in a 20-fold increase in CO formation, and in even higher CO concentrations with acetonitrile compared to the pure ionic liquid. Consequently, we propose that nitrile additives tune the interfacial structure in such a way that the access of water molecules is improved. In order to validate this hypothesis, we aim for an in-depth investigation of the bulk electrolyte as well as of the interfacial structure using *in situ* IR and SFG spectroscopy. [1] Ratschmeier et al. Electrochem. Sci. Adv. 2023, 3, e2100173.

O 34.6 Tue 13:30 P3

**Investigating Zinc Oxide-Water Interfaces with High-Dimensional Neural Network Potentials** — •Jan Elsner and Jörg Behler — Theoretische Chemie II, Ruhr-Universität Bochum, Germany, and ResearchCenter Chemical Sciences and Sustainability, Research Alliance Ruhr,Germany

Zinc oxide (ZnO) is a promising material for sustainable hydrogen production via catalytic water splitting. The interface of ZnO with water exhibits complex dynamical behavior, including water dissociation and recombination, as well as long-range proton transport. Traditionally, density functional theory (DFT)-based molecular dynamics has been the primary theoretical tool for probing such mechanisms at the atomistic scale. However, the complexity of the interface, requiring large simulation boxes, and the long time scales associated with dynamical processes pose substantial theoretical challenges for any method relying on explicit electronic structure calculations. High-Dimensional Neural Network Potentials (HDNNPs) offer a solution to these challenges, enabling atomistic simulations with DFT-level accuracy at only a fraction of the computational expense. Here, we present HDNNP-based simulations of ZnO-water interfaces, providing insights into their structure and dynamics.

## O 35: Poster Solid-Liquid Interfaces: Structure

Time: Tuesday 13:30–15:30 Location: P3

O 35.1 Tue 13:30 P3

**Comparision of spin and orbital Rashba effect in $Bi_xPb_{1-x}/Ag(111)$** — •Himanshu Lohani — EP7 University of Wurzburg

Superstructure of heavy elements constructed on the surface of noble metals is one of the most celebrated system in the field of spintronics due to giant Rashba spin splitting found in its surface electronic structure. A new perspective of orbitronics has emerged recently for reinvestigating this system after the uprising of orbital based Rashba effect. Angle resolved photoelectron spectroscopy (ARPES) not only visualizes directly the electronic band dispersion but intensity of the photoemission signal itself carries important information of orbital character of the bands. By using the photoemission intensity calculation which is designed on a tight binding model, we successfully capture evolution of the Rashba surface state bands (SSBs) dispersion and intensity as they are observed in our ARPES data on $Bi_xPb_{1-x}/Ag(111)$. This comparative study hints that buckling of Bi/Pb atoms on Ag(111) surface affects spin polarization of the Rashba SSBs more than their orbital polarization

O 35.2 Tue 13:30 P3

**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), a frequently used type of machine learning potential, have become a popular tool for simulations of complex systems such as mineral-water interfaces. Here, we present a HDNNP trained to density functional theory energies and forces for tricalcium aluminate ($Ca_3Al_2O_6$, $C_3A$)-water interfaces, which are of high interest for concrete chemistry. After validation, the obtained HDNNP is applied in large-scale molecular dynamics simulations to unravel the interactions of water with this material by computing a series of structural and dynamical properties.

O 35.3 Tue 13:30 P3

**Informed Automated Structure Discovery of Atomic Force Microscopy Images** — •Azin Alesafar[1], Joakim Jestilä[1], and Adam Foster[1,2] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Japan

Atomic Force Microscopy (AFM) enables direct imaging of atomic-level features however, the interpretation of non-planar molecules is challenging due to the fact that only the top layers of these systems interact with the microscope tip. This leads to images deviating from structures familiar to us. Recent Advances in machine learning-based image recognition tools have provided a framework suited to tackle this challenge. However, these methods rely heavily on training data and may produce inaccurate results when faced with unfamiliar structures. An alternative approach is to develop an iterative algorithm that generates realistic 3D structures by comparing simulated and experimental AFM images in a fully automated manner. The final workflow enables the generation of candidate structures using different techniques, such as molecular dynamics, minima hopping, or machine learning models. A deeper understanding of the simulated structural information is achieved through feature detection algorithms and image registration. Furthermore, the simulated structures, and consequently their corresponding AFM images, are automatically evaluated for similarity to reference AFM images using image quality metrics. These approaches are tested on water clusters modeled on gold and copper surfaces using the Neural equivariant interatomic potential (NequIP).

O 35.4 Tue 13:30 P3

**In situ electrochemical atomic force microscopy studies of a copper surface during lithium plating and dissolution** — •Luca Kaufer[1,2], Daniel Ebeling[1], Thomas Göddenhenrich[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 copper electrodes. In particular, the focus is on the deposition of lithium on copper surfaces, a crucial process in lithium batteries. Atomic force microscopy (AFM) measurements allow for precise analysis of the surface structure, morphology and dynamic changes during lithium deposition, thereby providing deeper insights into the mechanisms of electrode 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 include an examination of the modification of the single-crystal electrode surface, which has been achieved through the utilisation of a bespoke methodology that integrates sputtering, annealing and polishing techniques.

[1] J. Phys. Chem. C 2023, 127, 12492-12501. [2] Faraday Discuss, 2022, 233, 190.

# O 36: Poster 2D Materials: Electronic Structure and Exitations (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

O 36.1 Tue 13:30 P3

**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[1,3,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]Forschungszentrum Jülich — [3]TU Dresden — [4]Duke University, Durham, USA

In recent years, the emerging class of non-van der Waals 2D materials has attracted considerable interest due to the unique electronic and magnetic properties of the representatives [1]. We study here the role of spin-orbit coupling (SOC) in these non-van der Waals 2D systems and related effects that might eventually lead to topological properties. With several 2D candidates including heavy elements such as Bi and Tl, significant effects due to SOC are present in the electronic structure. For the initial screening, we employ AFLOW [2] with its standardized workflows. In a second step, we retrieve the metadata using AFLOW and adapt the extracted parameters with an AiiDA-plugin [3] for accurate electronic structure calculations using the full-potential all-electron program FLEUR [4] within AiiDA. We discuss the effect of SOC on the band structures and densities of states and also focus on the topologically protected 1D conduction edge channels [5].

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[2] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).
[3] G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016).
[4] The FLEUR project: https://www.flapw.de.
[5] M. Lokamani *et al.*, manuscript in preparation (2024).

O 36.2 Tue 13:30 P3

**Influence of surface relaxations on scanning probe microscopy images of the charge density wave material NbSe$_2$** — Nikhil S. Sivakumar[1], Joost Aretz[1], •Sebastian Scherb[1], Marion van Midden Mavric[2], Nora Huijgen[1], Umut Kamber[3], Daniel Wegner[1], Alexander A. Khajetoorians[1], Malte Rösner[1], and Nadine Hauptmann[1] — [1]IMM, Radboud University, Nijmegen, The Netherlands — [2]Jožef Stefan Institute, Ljubljana, Slovenia — [3]Joseph Henry Laboratories and Department of Physics, Princeton University, Princeton, USA

Scanning tunneling microscopy (STM) images of the charge density wave (CDW) in 2H-NbSe$_2$ at voltages around the Fermi level lack a contrast inversion expected for a single-band CDW. Recent works have ascribed this to a multiband CDW or the displacement of the surface Se atoms. While STM cannot disentangle geometric and electronic structure variations, non-contact atomic force microscopy (nc-AFM) can provide better characterization of the geometric structure due to its sensitivity to the interaction between the charge densities of tip and surface. We employ distance-dependent combined constant-height STM/nc-AFM measurements to characterize the surface relaxations of 2H-NbSe$_2$. Nc-AFM images show different image contrasts depending on distance. Based on ab-initio calculations, we show that the contrast at small distances is dominated by the displacement of the surface Se atoms. For large distances, the contrast is dominated by the interaction of the permanent dipole of the tip with the potential above the surface that is predominantly modulated by the underlying Nb atoms.

O 36.3 Tue 13:30 P3

**Investigation of the electronic structure of 1*T*-Ta$_{1-x}$Mo$_x$S$_2$ using 11eV-laser ARPES** — •Adina Timm[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

The ability to modify the electronic structure of quantum materials by controlling charge density waves (CDWs) offers various possibilities for use in next-generation technologies as electronic and optoelectronic components. A material platform for testing this approach is 1*T*-TaS$_2$, which exhibits different temperature-dependent CDWs that we aim to tune by doping. Using 11eV-laser ARPES, we determine the differences in the electronic band structure of both doped and pristine TaS$_2$ crystals. The dopant molybdenum was introduced into TaS$_2$ during crystal growth by chemical vapor transport. The photoemission results show that different CDW phases are present at low doping concentrations of less than one percent with modified transition temperatures.

O 36.4 Tue 13:30 P3

**Magnetic properties of V-doped WSe2** — •Jules M. Knebusch[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Florian K. Diekmann[1,2], Adina Timm[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

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 two-dimensional hexagonal $2H$ structure, is expected to transform into a room-temperature dilute ferromagnetic semiconductor upon vanadium doping, making it a highly attractive candidate for spintronic applications. This assumption is supported by density functional theory calculations and scanning transmission electron microscopy studies, and RKKY interactions are predicted as the driving mechanism. The crystals investigated in this study were synthesized in-house employing the chemical vapor transport method. This process produced as-is vanadium-doped $WSe_2$ crystals with approximately 2% of the tungsten atoms (presumably) substituted by vanadium. The results reported here were obtained using a Physical Property Measurement System (PPMS) in ACMS configuration and provide valuable insights into the magnetic characteristics of this doped material.

O 36.5 Tue 13:30 P3

**Polarons in single-layer MoS$_2$ via downfolding approach to the coupling of electronic and nuclear degrees of freedom** — •Laura Pätzold[1], Camiel van Efferen[2], Arne Schobert[1], Tfyeche Y. Tounsi[2], Michael Winter[1], Mark Georger[2], Affan Safeer[2], Christian Krämer[2], Jeison Fischer[2], Jan Berges[3], Thomas Michely[2], Roberto Mozara[1], Wouter Jolie[2], and Tim O. Wehling[1,4] — [1]U Hamburg — [2]U Köln — [3]U Bremen — [4]The Hamburg Centre for Ultrafast Imaging

A polaron is a quasiparticle describing a localized bound state resulting from the interaction of charge carriers with lattice vibrations. Though they are a well-studied phenomenon, experimental observations of polarons in 2D crystals are sparse. Here, we present the theoretical analysis of polaronic distortions in n-doped single-layer MoS$_2$ via a downfolding approach with linear electron-lattice coupling based on density functional theory calculations [1]. With this, a multi-polaronic distortion, caused by a renormalized M-point phonon, can be stabilized on supercells of up to $18 \times 18$. We compare our results to scanning tunneling microscopy measuremens obtained on n-doped single-layer MoS$_2$, which support the existence of polarons emerging from the coupling of non-polar zone-boundary phonons to Bloch electrons. This tunneling into the vibrationally coupled polaronic states is visible through evenly spaced peaks around the Fermi energy in the differential conductance, whose spacing matches the frequency of the M-point phonon responsible for the multi-polaronic distortion in our simulations.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)

O 36.6 Tue 13:30 P3

**Electronic and phononic characterization of 2H-NbS2 at the atomic scale** — •Werner M.J. van Weerdenburg, Margarete Huisinga, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDs) are a class of layered materials that can exhibit a variety of electronic properties, including low-temperature quantum phases such as superconductivity and charge density wave (CDW) formation. These phases may coexist, for instance in 2H-NbSe2, and electron-phonon interactions have been suggested as a common driving factor for the two phases [1]. In contrast, the similar compound 2H-NbS2 has a comparable superconducting critical temperature, but lacks a CDW phase [2], highlighting the importance of subtle differences in electron-phonon interactions.

Here, we apply scanning tunneling microscopy and spectroscopy (STM/STS) to investigate the electronic and phononic properties of 2H-NbS2 at the atomic scale. Based on quasiparticle interference mapping, we probe the spatial variation of the electronic density of states and identify the dispersion of the band structure around the Fermi level. Moreover, inelastic excitation spectroscopy reveals the phononic excitations of the material. By mapping the atomic-scale variation of phononic excitations around intrinsic defects of the material and adatoms, we study how electrons and phonons interact at the atomic scale.

[1] Rossnagel et al., PRB 64, 235119 (2001)
[2] Heil et al., PRL 119, 087003 (2017)

O 36.7 Tue 13:30 P3

**Characterization of surficial defect states in Mott insulator 1T-TaS$_2$** — •Junyoung Sim, Vibhuti Rai, Christian Lotze, and Katharina J. Franke — Freie Universtät Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

The Mott insulating state in 1T-TaS$_2$, arising from strong correlations among unpaired electrons within its charge density wave superlattice, is distinct from a trivial band insulator and serves as a model system for exploring the dynamics of exotic many-body states [1]. Here, we investigate bulk 1T-TaS$_2$ using scanning tunneling microscopy (STM) at 5 K. We find arious nanoscopic defects including vacancies, and domain. Additionally, we adsorb transition metal adatoms on the bare surface. Using tunneling spectroscopy, we map out their electronic signatures and compare them to prior studies [2].

[1] Hellmann et al. Phys. Rev. Lett. 105, 187401 (2010)
[2] Fei et al. AAPPS Bull. 32, 20 (2022)

O 36.8 Tue 13:30 P3

**FinEstBeAMS: a multipurpose VUV and soft X-ray beamline at the max iv laboratory** — •Weimin Wang, Antti Kivimäki, Kirill Chernenko, Calle Preger, and Stephan Appelfeller — MAX IV Laboratory, Lund University, PO Box 118, SE-22100 Lund, Sweden

The Finnish-Estonian Beamline for Atmospheric and Materials Science (FinEstBeAMS), located at the 1.5 GeV storage ring of the MAX IV Laboratory (Lund, Sweden), is a multidisciplinary beamline that was designed to fulfil the various needs of scientific communities in atomic, molecular and optical research, surface science, and photoluminescence research.

The gas-phase end station is equipped for electron and time-of-flight ion spectroscopies in low-density matter, while the photoluminescence end station focuses on luminescence spectroscopy of solid samples. The solid-state end station is dedicated to photoelectron and X-ray absorption spectroscopy of surfaces and interfaces, utilizing a hemispherical electron energy analyzer (PHOIBOS 150 2D-DLD from SPECS). The sample is positioned via a 5-axis motorized manipulator, offering three linear and two rotational motions (polar and azimuthal). A cryostat integrated into the manipulator enables sample cooling with liquid helium (~50 K) and nitrogen (~90 K). Additionally, a preparation chamber allows for sample treatment and analysis using supplementary techniques.

# O 37: Poster 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

O 37.1 Tue 13:30 P3

**Two-dimensional hexagonal $\beta$-GeSe on Au(111)** — •Dina Wilks, Veronika Blecker, Muhammad Ali Martuza, Marina Hammer, Christoph Schuster, Paulus Aleksa, and Carsten Busse — Walter-Flex-Straße 3, 57072 Siegen, Germany

Two-dimensional (2D) group-IV monochalcogenides (general form MX with M=Sn, Ge; X=S, Se, Te) demonstrate a high degree of polymorphism. While the orthorhombic phase, widely studied for its inplane ferroelectricity, holds significant promise, experimental studies on other polymorphs remain scarce.

Here, we investigate the growth and structure of 2D hexagonal $\beta$-GeSe on Au(111). This phase is predicted to exhibit out-of-plane ferroelectricity, which could be more technologically feasible for device integration. Samples are prepared using molecular beam epitaxy (MBE) with GeSe powder as the source material and analyzed with low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). The degree of structural order was found to depend sensitively on the heat treatment. We observe a $(5 \times 5)$ superstructure relative to Au(111), accompanied by a continuously varying density of states (DOS) across the superstructure's unit cell. Additionally, an intriguing self-similar pattern emerges, which can be attributed to antiphase grain boundaries. These boundaries exhibit metallic behaviour near the Fermi level, highlighting their potential significance in the electronic properties of the system.

O 37.2 Tue 13:30 P3

**Scanning Tunneling Microscopy and Spectroscopy of epitaxial grown TaS$_2$ on GaN (0001)** — •Jan-Niclas Schmidt, Constantin Hilbrunner, Georg A. Traeger, Jörg Malindretos, Angela Rizzi, and Martin Wenderoth — University of Göttingen, IV. Physikalisches Institut, Fridrich-Hund-Platz 1, 37077 Göttingen

Tantalum Disulfide crystals are interesting due to its complex phase diagram including the effect of Charge Density Waves. We are interested in how the layer thickness influences properties of Tantalum Disulfide. With Molecular Beam Epitaxy a three monolayer thick film of 2H-Tantalum Disulfide was grown on Gallium Nitride. To gain insight into the growth mechanism, the sample was transferred to a low temperature Scanning Tunneling Microscope (STM) operated at 80 K. To avoid any surface contamination, the transfer was done with a portable ultrahigh vacuum chamber. The constant-current STM-topography show small nanometer-sized, trigonal islands on a rough layer with some holes. The spectroscopy data show metallic behavior for the island as well as for the layer below.

This work is financially supported by the DFG through the SFB1073.

O 37.3 Tue 13:30 P3

**Growth dynamics of 2D materials on Ir(111)** — •Smruti Ranjan Mohanty, Marko Kriegel, Frank Meyer zu Heringdorf, and Michael Horn- von Hoegen — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany

The structure and morphology of 2D materials are profoundly influenced by the choice of growth substrates, with noble metal substrates offering enhanced catalytic activity and complex surface morphology facilitating precise control over the growth of 2D materials. Employing low-energy electron microscopy (LEEM), we investigated the kinetics of graphene island nucleation during the CVD of ethylene on Ir(111) at growth temperatures ranging from 750°C to 1050°C for various dosing pressures. Graphene islands nucleate heterogeneously at Ir(111) step edges, leading to edge decorations, but a transition to homogeneous nucleation occurs at island densities lower than the step density. The strong variation in island density as a function of growth temperature and dosing pressure is explained by Venables nucleation theory, with the near-linear dependence on dosing pressure attributed to a critical nucleus size (i*) of 5. The work presented here also extends to the growth and characterization of other atomically thin 2D materials, including hexagonal boron nitride (hBN), and borophene on Ir(111). The investigation reveals complex growth mechanisms, the emergence of Moiré superlattices, and substrate-influenced interactions, providing insights for designing heterostructures and functional materials with significant potential for next-generation technological applications.

O 37.4 Tue 13:30 P3

**Incommensurability and negative thermal expansion of single-layer hexagonal boron nitride** — •Marko Kriegel[1], Karim Omambac[1], Steffen Franzka[2], Frank Meyer zu Heringdorf[1,2], and Michael Horn-von Hoegen[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Interdisciplinary Center for Analytics on the Nanoscale (ICAN), Carl-Benz-Str. 199, 47057 Duisburg, Germany

The emerging field of straintronics, i.e., the control and utilization of the strain state of 2D-materials, is of great importance for their technological development, specifically in view of their future incorporation into van der Waals heterostructures. To gain fundamental insight into structural peculiarities of two-dimensional systems, single-layer hexagonal boron nitride (hBN) grown on Ir(1 1 1) by chemical vapor deposition was used as a prototypical model system: High-resolution reciprocal space mapping reveals the incommensurate nature of the material system by measuring the *h*BN in plane lattice parameter with high precision, facilitated by the moiré magnification effect in electron diffraction. In a growth temperature ($T_g$) regime of 700 to 1150°C an average lattice parameter of $2.496 \pm 0.006$ Å was found. Eventually, careful disentanglement of the hBN and substrate behavior for rising $T_g$ allowed the determination of a negative thermal expansion coefficient of $\alpha_{\mathrm{hBN}} = 2.4 \pm 1.2 \times 10^{-6}\,\mathrm{K}^{-1}$ for free-standing hBN.[1] [1] M. Kriegel et al. Appl. Surf. Sci. 624 (2023) 157156

O 37.5 Tue 13:30 P3

**UHV-CVD on Ir(111) for the Growth of 2D Materials** — •Niels Ganser[1], Marko Kriegel[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], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen — [2]Institute of Physics, Zagreb — [3]ICAN, Duisburg — [4]Universität zu Köln

Hexagonal boron nitride (hBN) can be grown by scalable chemical vapor deposition (CVD) from a borazine $B_3N_3H_6$ precursor. Here we show that the hBN quality depends strongly on the growth temperature $T_g$ and the dosing pressure $p$.

Combined SPA-LEED and LEEM measurements show a strong dependence of $n$ on $p$. We find that the quality of the hBN layers that can be achieved by increasing $T_g$ is limited by the process of disintegration of the borazine at $T_g > 950\,^\circ$C resulting in growth of borophene (2D Boron) instead [1]. Thus, it is possible to selectively grow either hBN or borophene from the same precursor [2].

Corroborating SPA-LEED measurements reveal a negative thermal expansion coefficient of $\alpha = (-2.4 \pm 1.2) \times 10^{-6}\,\mathrm{K}^{-1}$ for 2D hBN in the temperature regime between 700 and 1100 °C. This finding can be explained by Lifshitz' membrane effect [3].

[1] Lifshitz, I., Zh. Eksp. Teor. Fiz. 22, 475 (1952)
[2] Omambac, K. et al., ACS Nano 15, 7421 (2021)
[3] Omambac, K. et al., ACS Nano 17, 17946 (2023)

## O 38: Poster 2D Materials: Stacking and Heterostructures (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

O 38.1 Tue 13:30 P3

**Stability and electronic properties of double-layer o-B2N2 in different stacking modes** — •Na Li and Claudia Draxl — Department Physics and CSMB, Humboldt-Universit at zu Berlin, D-12489 Berlin, Germany

Two-dimensional orthorhombic boron nitride (o-B2N2) has recently attracted significant attention due to its direct band gap of approximately 1.7eV and excellent visible-light absorption properties. In its layered conformations, the stacking order plays a crucial role in determining the material's stability as well as its electronic and optical properties. In this study, we employ the all-electron full potential code exciting to perform first-principles calculations of four high-symmetry bilayer stacking sequences of o-B2N2, regarding their relative stability and their electronic properties. Our calculations reveal that the AB' stacking sequence has the lowest energy and an optimized interlayer distance of 3.52 Å. The bandgaps of the AA and AA' stacking sequences are reduced relative to the monolayer, where AA' exhibits even semi-metallic behavior. In contrast, the AB and AB' stacking sequences show slightly increased direct bandgaps.

O 38.2 Tue 13:30 P3

**In-depth analysis of stratified MoS2 and WS2 2D heterostructures** — •Sebastian Klenk, Nikolas Dominik, Cormac Ó Coileáin, Tanja Stimpel-Lindner, and Georg S. Duesberg — University of the Bundeswehr Munich, Institute of Physics, Germany

Starting with graphene roughly two decades ago, two-dimensional (2D) materials have garnered great interest in the scientific community due to their exceptional electrical, mechanical and optical properties. The broad palette of different 2D materials has allowed for the possibility to change and finetune these parameters to one's own liking by combining several 2D materials in one film. Here, we present the metal-organic chemical vapour deposition (MOCVD) synthesis and analysis of MoS2/WS2 heterostructures. We show the ordering of a high-quality 7-layer combination structure of less than 10 nm. The layered nature is confirmed and discussed using XPS, EDX, ToF-SIMS, TEM, AFM and Raman spectroscopy.

O 38.3 Tue 13:30 P3

**A Two-dimensional Heterostructure Fabrication System in Ultra-high Vacuum** — •Daiyu Geng, Jiabao Yang, Natalie Lehmann, and Niels Schröter — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle (Saale), Germany

We develop an ultra-high vacuum system for the fabrication of two-dimensional heterostructures. The clean transfer and stacking of two dimensional material flakes are realized using a polymer-free method based on SiNx cantilevers coated with Au film (Nature Electronics, 2023, 6(12): 981-990). The system also incorporates multiple surface preparation and characterization techniques like MBE, Plasma sputtering and electron diffraction. All these methods enable us to prepare heterostructures with atomically clean interface, which is important for the spectroscopic investigation of the rich physics effects in two-dimensional heterosystems.

O 38.4 Tue 13:30 P3

**Exploring MXenes as Electrodes for Al-ion Batteries: An Ab-initio Study on the Impact of Stacking Configurations and Termination Types** — •Amal Raj Veluthedath Nair and Nuala M Caffrey — School of Physics, University College Dublin, Dublin 4, Ireland

MXenes, with their tunable surface chemistry, thin 2D structures, large interlayer spacing, and good conductivity, are promising candidates for battery electrodes. The stacking configuration of MXene layers, determined by their chemistry and surface terminations, influences their electrochemical performance.

This study explores $Ti_3C_2$ and $V_2C$ MXenes as electrodes for Na, Mg, and Al-ion batteries using density functional theory. We examine four stacking configurations and two coordination sites for intercalated ions. Results reveal that stacking configuration and surface terminations significantly influence change in interlayer distance, with O-terminated octahedral stacking showing the least change in spacing for all intercalants. The smallest interlayer distance change occurs for Al intercalation in $V_2C$, with a $\Delta$d of 0.1 Å, matching experimental findings (Vahidmohammadi et al., 2017). Ion migration studies indicate that prismatic stacking promotes faster ion migration compared to octahedral stacking. O-terminated MXenes significantly enhance the theoretical specific capacity for Al intercalation, reaching a maximum value of 283.48(277.63)mAh/g for $Ti_3C_2O_2$($V_2CO_2$). In contrast, F-terminated MXenes show much lower capacities.

O 38.5 Tue 13:30 P3

**Triplet pairing enabled proximity superconductivity in monolayer WTe$_2$** — •A. Bäder[1,2], T. Wichmann[1,3], J. Martinez-Castro[1,4], P. Rüssmann[5,6], K. Jin[1,4], T. Samuely[7], Z. Lyu[1,3], J. Yan[8], O. Onufriienko[7], P. Szabó[7], F. S. Tautz[1,3], M. Ternes[1,4], S. Lounis[5,9], and F. Lüpke[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]II. Physikalisches Institut, Universität zu Köln — [3]Institut für Experimentalphysik IV A, RWTH Aachen — [4]Institut für Experimentalphysik II B, RWTH Aachen — [5]Peter Grünberg Institut (PGI-1), Forschungszentrum Jülich — [6]Julius-Maximilians-Universität Würzburg, Fakultät für Physik und Astronomie — [7]Centre of Low Temperature Physics, Faculty of Science, Pavol Jozef Šafárik University & Institute of Experimental Physics, Slovak Academy of Sciences — [8]Materials Science and Technology Division, Oak Ridge National Laboratory, USA — [9]Fakultät für Physik, Universität zu Duisburg-Essen

We use low-temperature scanning tunneling microscopy to investigate proximity-induced triplet pairing and its role in enabling superconductivity in a monolayer $WTe_2/NbSe_2$ van der Waals heterostructure. Employing the Kohn-Sham Bogoliubov-de Gennes formalism, we find that conventional s-wave pairing fails to induce superconductivity in the $WTe_2$, in contrast to triplet pairing. Applying an external magnetic field, we examine Abrikosov flux vortices within the heterostructure and exploit them to probe local superconducting properties. Our findings highlight a platform for studying triplet pairing-induced superconductivity with potential topological characteristics.

## O 39: Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules I

Time: Tuesday 14:00–15:30 Location: H4

O 39.1 Tue 14:00 H4

**Instrumental Innovations for Model Single-Atom Catalysis** — •Jiří Pavelec, David Rath, Chunlei Wang, Nail Barama, Panukorn Sombut, Matthias Meier, Michael Schmid, Ulrike Diebold, and Gareth S. Parkinson — TU Wien, Vienna, Austria

Single-atom catalysts (SACs) reduce reliance on precious materials by using individual atoms as active sites. Infrared spectroscopy of adsorbed CO is widely used to probe these sites, but spectral interpretation and charge-state assignment remain debated. Surface science studies of model SACs could provide valuable benchmarks, but progress has been hindered by a lack of model systems and challenges in detecting low coverages of intermediates.

Here, I introduce a novel approach to infrared reflection absorption spectroscopy (IRAS) that adjusts the incidence angle, which resolves signal-to-noise issues on dielectrics [1]. As a case study, we investigated CO titration of rhodium-based SACs on a $Fe_3O_4(001)$ support. The spectra reveal $Rh_1CO$ monocarbonyls as the dominant species. Meanwhile, the $Rh_1(CO)_2$ gem-dicarbonyl arises solely from the breakup of minority $Rh_2$ dimers, as confirmed by STM movies and theoretical modeling [2]. Though less prevalent in our UHV study, $Rh_1(CO)_2$ may play a critical role under realistic conditions.

Combining advancements in IRAS with a detailed understanding of model SACs provides valuable benchmarks for theoretical studies and spectral references for researchers working with less-defined, high-surface-area powder catalysts. [1] D. Rath et al., Rev. Sci. Instrum. 95, (2024). [2] C. Wang et al., Angew. Chem. Int. Ed. 63, (2024).

O 39.2 Tue 14:15 H4

**Structure and oelic acid adsorption properties of magnetite nanoparticles on $SrTiO_3$** — •mohammad ebrahim haji naghi tehrani[1,2], lucio martinelli[3], daniel silvan dolling[1,2], marcus creutzburg[1], ming chao kao[1,2], alexander meinhardt[1,2], mona kohantorabi[1], heshmat noei[1], and andreas stierle[1,2] — [1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [2]Fachbereich Physik Universität Hamburg, Hamburg, Germany — [3]Institut Néel, CNRS, Grenoble INP, Université Grenoble Alpes, Grenoble, France

The underlying explanation for the exceptional mechanical properties of hierarchically arranged magnetite nanoparticle super-crystals is closely linked to understanding the oxide-organic interface between the magnetite nanoparticles (NPs) and the oleic acid (OA) molecules. We studied the shape and surface structure changes of the magnetite NPs induced by crosslinking the OA molecules. In this regard, magnetite NPs were grown by reactive physical vapor deposition on a strontium titanate single crystalline surface (STO(001)). The structural and morphological changes in the NPs were monitored under ultra-high vacuum (UHV) conditions employing synchrotron-based grazing incidence X-ray diffraction (GIXRD). We evidenced the growth of (001) oriented magnetite NPs with predominant (111) side facets. Additionally, our results indicate an increase in the NP lattice constant after OA adsorption, which may be attributed to the incorporation of oxygen vacancies.

O 39.3 Tue 14:30 H4

**Towards Understanding the Photoreactivity of $SrTiO_3$ through Studies in Ultra-High Vacuum** — •Anna Lemperle, Philip Petzoldt, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Heterogeneous photocatalysis offers the prospect of utilising solar energy for the zero-carbon production of hydrogen from water. The most prominent photocatalytic materials currently employ $SrTiO_3$ as the light harvesting semiconductor. While these catalysts have been shown to promote a stoichiometric reaction, their photocatalytic performance is still insufficient for economically viable application. As their structural complexity impedes mechanistic studies, model systems are necessary to elucidate individual reaction steps and connect catalytic results to distinct catalyst properties. This approach aims to attain a molecular understanding of the reaction mechanisms involved in water splitting in order to enable a more targeted design of photocatalysts. In this contribution, we discuss first results on the reactivity of water and oxygen on the bare $SrTiO_3(110)$ surface. Results obtained by combining temperature programmed desorption and studies under illumination highlight the importance of bulk and surface oxygen for the reactivity of $SrTiO_3$.

O 39.4 Tue 14:45 H4

**Effect of Mn and V Doping on the OER activity of $Co_3O_4(001)$: insights from DFT+$U$ calculations** — •Palani Muthu Kumar and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

Using density functional theory calculations with a Hubbard $U$ term (DFT+$U$), we study the effect of Mn and V doping on the oxygen evolution reaction (OER) at the $Co_3O_4(001)$ surface. In bulk, both dopants favor the octahedral over the tetrahedral site, providing a foundation for understanding the incorporation at the surface. Both at the A and the B-terminations of $Co_3O_4(001)$, Mn doping at a surface octahedral site enhances the overpotential, reducing overall the OER efficiency. In contrast, at the B-layer, V doping at a surface octahedral site reduces the overpotential from 0.48V (pristine) to 0.43 V, retaining the $Co_{oct}$ reaction site. At the pristine A-surface, $\eta$ is higher for a tetrahedral (0.74 V) vs. octahedral surface Co site (0.55 V). This trend is reversed for V-doping in the subsurface octahedral site which leads to the lowest overpotential of 0.18 V at the $Co_{tet}$ reaction site. In all studied cases, the potential determining step is the deprotonation of *OH to *O. The improved catalytic activity due to V doping is attributed to a modified charge redistribution on the surface, leading to favorable binding energies of the intermediates. Funding by DFG within CRC247 and computational time at the Leibniz Rechenzentrum are gratefully acknowledged.

O 39.5 Tue 15:00 H4

**Complex structural arrangements at the $CO_2/In_2O_3(111)$ interface** — Sarah Tobisch[1], Andreas Ziegler[2], Marco Knapp[1], Michael Schmid[1], Ulrike Diebold[1], Bernd Meyer[2], and •Margareta Wagner[1] — [1]Institut für Angewandte Physik, TU Wien — [2]ICMM & CCC, FAU-Erlangen-Nürnberg

Promising catalysts for the hydrogenation of $CO_2$ to methanol are highly desired to address the pressing issue of rising carbon emissions. Since reactions take place at the interface, understanding the fundamental properties and behavior of molecular species on well-defined surfaces is crucial for designing model catalysts.

$In_2O_3$ has gained attention as catalytic material due to its high selectivity for methanol synthesis via $CO_2$ reduction. In this work, the adsorption and interaction of $CO_2$ molecules on $In_2O_3(111)$ were investigated in detail at the atomic scale and under UHV conditions. We employ non-contact atomic force microscopy (AFM) and compared our findings with results from temperature programmed desorption (TPD) and x-ray photoelectron spectroscopy (XPS) measurements, as well as density functional theory (DFT) calculations. AFM images of the $In_2O_3(111)$ surface show 10 molecular features per surface unit cell arranged in a systematic and uniform order, albeit breaking the threefold symmetry of the substrate surface. The adsorption sites of all individual molecules were identified; some of them are carbonate species, in agreement to XPS showing a mixture of $CO_2$ molecules and $CO_3^{2-}$. Moreover, the desorption and structural evolution with increasing temperature was studied.

O 39.6 Tue 15:15 H4

**Adsorption and activation of $CO_2$ on $CeO_2$ surfaces** — •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

CO$_2$ activation and its subsequent transformation into valuable chemicals pose significant challenges in heterogeneous catalysis. Most studies have focused on powdered catalysts with various facets and unknown defect densities, whereas much less is known about the surface chemistry of CO$_2$ on well-defined oxide surfaces. Here, we investigate CO$_2$ adsorption and activation on fully oxidized CeO$_2$(111) single-crystal surfaces using polarization-resolved IR reflection absorption spectroscopy (IRRAS). The comprehensive IRRAS data reveal that CO$_2$ is weakly bound to CeO$_2$(111) at 117 K in a linear, physisorbed state. At elevated temperatures (300 K) and pressures, CO$_2$ undergoes activation forming an unusual horizontal carbonate. Additionally, in the presence of surface hydroxyl groups, formate and HCO$_3$ species are identified. These experimental findings are supported by complementary theoretical analysis. Furthermore, the IRRAS results are in excellent agreement with the in situ transmission IR data obtained for CO adsorption on octahedral ceria nanoparticles, which predominantly expose (111) facets. This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) -Project-ID 426888090- SFB 1441.

## O 40: Surface Dynamics

Time: Tuesday 14:00–15:30 Location: H6

O 40.1 Tue 14:00 H6

**Manipulation of Optical Phonons in Strained Bi/Si(001) Heterostructures** — •Fabian Thiemann and Michael Horn-von Hoegen — University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Intentionally manipulating phononic properties in materials can cause dramatic changes in their dynamic behavior. A system that responds especially strong to structural changes is Bi due to its strong electron-phonon coupling and its inherent Peierls distortion. This renders the optical $A_{1g}$ mode – oscillating along the [111] direction – sensitive to changes in the electronic system and coherently excitable upon photoexcitation. When grown on Si(001) bismuths lattice matches in the [$1\bar{1}0$] direction, resulting in a compressive strain in the [110] direction, whereas the films are [111] oriented. The strain is relieved rapidly while increasing the thickness from 10 to 16 BL. This is predicted to influence the Peierls distortion heavily. In this work we extensively studied the impact of strain and confinement on the photoexcited coherent $A_{1g}$ mode's frequency and dephasing in Bi/Si(001) heterostructures by in-situ transient-reflectivity spectroscopy. We observe a dramatic blueshift up to 0.2 THz, that can be preciesely tuned by the film thickness. The frequency however does not follow exactly the strain parameter and behaves differently in two regiemes. We attribute this discrepancy to the confinement in the [111] direction and the influence of the strongly shifting electron surface state.

O 40.2 Tue 14:15 H6

**Coherent modulation of the charge density wave gap in 1T-TiSe$_2$ probed by tr-ARPES** — •Jan Böhnke, Stephan Schmutzler, Mehul Jotshi, Cornelius Gahl, and Martin Weinelt — Freie Universität Berlin, Fachbereich Physik, Germany

Tuning the charge density wave (CDW) gap in 1T-TiSe$_2$ allows for the de/stabilization of the phase transition. An optical excitation breaks long-range order of the CDW state and results in a semi-metallic state on an ultrafast timescale as free carriers near the Fermi-level enhance Coulomb screening [1,2]. By employing time-resolved ARPES with 1.55 eV pump and 6.2 eV probe pulses, we discover for the first time fluence-dependent coherent modulations of the charge-density wave gap (closing and opening) in 1T-TiSe$_2$ at the Brillouin zone center. While for low excitation fluences, we mainly observe signatures of the CDW connected $\mathrm{A}^*_{1\mathrm{g}}$ mode (3.45 THz), the optical $\mathrm{A}_{1\mathrm{g}}$ phonon mode (6.1 THz) modulates the electronic structure near the gap for the high fluence regime. For an intermediate fluence we detect the transition from the $\mathrm{A}^*_{1\mathrm{g}}$ to the $\mathrm{A}_{1\mathrm{g}}$ mode. As we additionally find three image-potential states on the surface of 1T-TiSe$_2$, we can confirm the samples' low defect density at the surface after in-vacuum cleavage.

[1] T. Rohwer et al., Nature 471, 490–493 (2011)

[2] M. Huber et al., Sci. Adv. 10, eadl4481(2024)

O 40.3 Tue 14:30 H6

**Impact of Coherent Phonons on Time-Resolved Optical Properties of WTe$_2$** — •Francesco Sammartino[1], Manuel Tuniz[1], Wibke Bronsch[2], Fulvio Parmigiani[1,2], and Federico Cilento[2] — [1]Università degli Studi di Trieste — [2]Elettra - Sinctrotrone Trieste

We study the ultrafast dynamics of tungsten ditelluride (WTe$_2$) along both its in-plane axes, by time-resolved reflectivity (TR-R) and time-resolved second-harmonic generation (TR-SHG) experiments with a varying pump fluence.

We identify two phonon modes: the shear phonon mode at 0.24 THz, indicative of uniform in-plane atomic shifts and detected in both TR-R and TR-SHG signals, and one at 2.4 THz, detected solely in the TR-R signal. We observe a large, fluence-dependent shift of up to ≈90° in the initial phase of the shear mode coherent oscillation, obtained in a narrow fluence range.

This evidence suggests that the excitation density can be used as a powerful knob to control the initial phase of the atomic displacements in a layered material.

O 40.4 Tue 14:45 H6

**Controlled formation of thermodynamically unaccessible surface structures** — •Simon B. Hollweger, Anna Werkovits, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Austria

It is well known that organic molecules adsorbed on surfaces can form a variety of different surface structures. Which structure is the most favored one at a given temperature and pressure is determined by thermodynamics. However, in this study, we propose the idea of a mechanism with which we can control the formation of a specific metastable surface polymorph that can not be reached thermodynamically. With targeted temperature and pressure changes, a rearrangement process of the adsorbed molecules out of thermodynamic equilibrium is triggered. For specifically designed systems, this rearrangement of the adsorbed molecules leads to a kinetically trapped metastable surface polymorph. As a proof of principle for this proposed mechanism, kinetic Monte Carlo simulations of planar molecules adsorbing on a square lattice are conducted. We show that a metastable upright-standing structure of the planar molecules can be reached with a specific temperature and pressure profile applied to the system.

O 40.5 Tue 15:00 H6

**Out of the Crystalline Comfort Zone: Sampling the Initial Oxide Formation at Cu(111)** — •Felix Riccius, Nicolas Bergmann, Hendrik H. Heenen, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

The oxidation of transition metal surfaces is widely recognized as a complex process that still bears many open questions, specifically at the microscopic level. Atomistic simulations could potentially uncover crucial insights, but state-of-the-art approaches are predominantly guided by human chemical intuition, leading to highly idealized surface representations. Here we demonstrate a systematic approach to model high-quality surface-phase diagrams, using the early oxidation of the Cu(111) surface as an example. To this end, we train a MACE machine learning interatomic potential (MLIP) to density functional theory calculations and combine its fast and accurate energetics with replica exchange molecular dynamics. We extensively explore the vast, thermodynamically relevant phase space and further develop surface phase diagrams based on increasingly involved theoretical frameworks. Our approach yields a comprehensive structural ensemble that predicts early Cu(111) oxidation to be characterized by O-Cu-O ring patterns, bearing significant disorder. Within the computed surface evolution, we recover trends in O-Cu-O ring distribution as a function of reaction conditions in line with scanning tunneling microscopy data. Our study illustrates how MLIPs and extensive sampling can be leveraged to rationalize metal surface oxidation fully *in silico* without the need to rely on experimental guidance.

O 40.6 Tue 15:15 H6

**Photo-induced carrier and structural dynamics in anatase**

**$TiO_2$ nanosheets** — •Zhipeng Huang[1,2], Yan Yan[2], Xinxin Cheng[2,3], R. J. Dwayne Miller[4], and R. Kramer Campen[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen — [2]Max Planck Institute for the Structure and Dynamics of Matter — [3]SLAC National Accelerator Laboratory — [4]Departments of Chemistry and Physics, University of Toronto

Ultrathin anatase $TiO_2$ nanosheets with $\{001\}$ facets have significantly higher activity for light-induced $H_2$ evolution than other $TiO_2$-based materials. The mechanism of this enhancement is not understood. Gaining such insight requires understanding the dynamics of charge carriers and their interactions with lattices after optical excitation. Here we characterize structural and charge carrier dynamics in these materials following UV excitation using ultrafast electron diffraction and transient absorption spectroscopy.

We observed an ultrafast lattice expansion and distortion in the nanosheets, occurring earlier than the Debye-Waller effect. Density Functional Theory (DFT) calculations suggest that the lattice expansion and distortion are induced by the trapping of charge carriers and the formation of large electron polarons. Compared to $TiO_2$ nanoparticles, the nanosheets exhibit significantly higher polaron populations, which explains their enhanced photocatalytic properties.

## O 41: Heterogeneous Catalysis II

Time: Tuesday 14:00–15:15 Location: H8

O 41.1 Tue 14:00 H8

**Oxide growth and oxide/metal interaction in $CeO_x$/Ni(111)** — •Dominic Guttmann, Raquel Sánchez-Barquilla, Carlos Morales, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Cottbus 03046, Germany

Ni/ceria catalysts exhibit a high activity and selectivity for $CO_2$ methanation, making them very promising candidates for applications within a sustainable economy. The redox properties of cerium oxide allow it to readily switch between $Ce^{4+}$ and $Ce^{3+}$ states, facilitating $CO_2$ activation and conversion. We have studied the so-called strong metal-metal oxide interactions in the inverse catalyst configuration $CeO_x$/Ni(111) prepared by reactive molecular beam epitaxy in an oxygen atmosphere. Under specific growth conditions, the $CeO_x$ (111)-oriented islands of different heights preferentially align in registry with the Ni(111) surface or are rotated azimuthally by ±10°, as observed by low-energy electron diffraction. Analysis by X-ray photoelectron spectroscopy reveals that during growth, partial oxidation of the Ni(111) surface leads to the formation of a NiO interface layer between the $CeO_x$ islands and Ni substrate, resulting in a complex $CeO_x$(111)/NiO(111)/Ni(111) system with significant oxide-metal interactions. Finally, when we expose the system to $H_2$, $O_2$, and $CO_2$ atmospheres, we observe a complex behavior of the cerium and nickel oxidation states, which correlate with morphological changes in the oxide islands.

O 41.2 Tue 14:15 H8

**Size-dependent nanoparticle sintering under catalytic reaction conditions** — •Thomas Florian Keller[1,2], Christoph Seitz[1], Henning Runge[1], Vedran Vonk[1], and Andreas Stierle[1,2] — [1]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]University of Hamburg, Department of Physics, Hamburg, Germany

Catalytic metal nanoparticles applied in heterogeneous gas phase catalysis are known to change their shape during the conversion. We elucidate the evolution of the height to diameter aspect ratios of a substantial number of PtRh alloy nanoparticles exposed to mild and harsh catalytic CO oxidation reaction conditions by correlative atomic force- and scanning electron-microscopy. The preferentially (111) oriented Pt rich nanoparticles supported on a (0001) $Al_2O_3$ single crystal surface were imaged as grown and after the exposure to the catalytic conditions. We utilized an image-registration based approach combined with one-by-one nanoparticle correlation to overcome single nanoparticle studies and ensemble averages. This approach permitted us to shed light onto the active size dependent sintering mechanism as e.g., particle migration and coalescence, and Ostwald ripening. While for mild catalytic conditions the aspect ratio is rather independent of the lateral nanoparticle size, for harsh conditions particles above an initial threshold diameter of around 45 nm tend to extraordinary grow on the cost of the surrounding smaller particles.

O 41.3 Tue 14:30 H8

**High-throughput photocatalytic screening of lead-free halide perovskites with bayesian optimization for surface photovoltage** — •Astita Dubey[1,2], Mahshid Ahmadi[2], Vladimir Shvartsman[1], Sergei Kalinin[2], and Doru Lupascu[1] — [1]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstr. 15, 45141 Essen, Germany — [2]Institute for Advanced Materials and Manufacturing, Department of Materials Science and Engineering, The University of Tennessee Knoxville, Knoxville, TN 37996, USA

The development of lead-free, stable, and efficient catalysts for energy conversion necessitates rapid materials discovery. In this study, we employed Bayesian optimization (BO) to investigate a one-dimensional binary combinatorial library of zero-dimensional lead-free halide perovskites (A3Bi2I9 types) synthesized using a high-throughput automated pipetting robot. Structural analysis revealed hexagonal P6*/mmc symmetry throughout the library with pronounced variations in the lattice parameter c. Gaussian process-based BO identified the optimal composition featuring 49% cesium substitution, which demonstrated the best photocatalytic activity and stability attributed to the enhanced surface photovoltage and optimized anion vacancies. This composition achieved complete degradation of rhodamine B and methylene blue dyes within 15 and 20 minutes, respectively. The identified composition's stability, defect management and the most efficient photocatalytic activity among 96 compositions is promising for its further use in water splitting.

O 41.4 Tue 14:45 H8

**Automatic Exploration of Catalytic Reaction Networks** — •Hyunwook Jung, Johannes T. Margraf, Hendrik H. Heenen, and Karsten Reuter — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195, Berlin

The reaction network is a crucial element of first-principles microkinetics simulations, representing the connection between surface species and elementary reactions. Lacking systematic exploration methods, the reaction network is presently typically set up by human intuition. Especially for complicated processes such as syngas conversion, this is error prone and the absence of important species and reaction steps can be a source of sizable discrepancy between theoretical modeling and experiment. To address this problem, we introduce an automatic reaction network exploration scheme that starts with a fully enumerated, yet redundant reaction network, in which a reaction pathway is refined iteratively. The associated computational cost for extensive sampling of structures for both adsorption and activation energy calculations along the pathway is circumvented by simultaneously fine-tuning a MACE foundation model. Each trial reaction pathway is coupled with corresponding mean-field microkinetics and a detouring operation is attempted for the identified rate-limiting step. This procedure is repeated until user-defined criteria are reached. We demonstrate this automatic scheme on methanol synthesis at a Cu(111) surface.

O 41.5 Tue 15:00 H8

**Functionalization of atomically defined Au step edges with N-heterocyclic carbenes for the electrocatalytic reduction of carbon dioxide** — •Philipp Wiesener[1], Duong Tran[1], Ankita Das[2], Ying Pan[3], Nieves Lopez Salas[3], Frank Glorius[2], and Harry Mönig[1] — [1]Physikalisches Institut, Universität Münster, Münster, Germany — [2]Organisch-Chemisches Institut, Universität Münster, Münster, Germany — [3]Institut für Chemie, Universität Paderborn, Paderborn, Germany

N-Heterocyclic carbenes (NHCs) are versatile ligands allowing to tune the catalytic performance of metal surfaces and nanoparticles. In recent years, the understanding of molecular adsorption of a variety of NHC compounds on flat single crystalline surfaces has significantly advanced the knowledge about their extraordinary properties. In the present work, we use scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) to investigate the adsorption of various NHCs on a Au(788) surface, featuring a high density of atomically defined step edges. Our results reveal that NHC nucleation is significantly more stable at the step edges than on flat terraces. Correlating sub-molecular imaging techniques with voltammetry, we demonstrate the formation of a macroscopically defined and catalytically active nanostructure for the $CO_2$ reduction reaction. Our results spotlight the important role and opportunities of step edge functionalization by NHC compounds to design highly efficient and selective catalysts with defined active sites.

## O 42: Electron-driven Processes

Time: Tuesday 14:00–15:30 Location: H11

O 42.1 Tue 14:00 H11

**A simple model of nonadiabatic energy loss during hydrogen scattering from a semiconductor** — •Xuexun Lu, Nils Hertl, and Reinhard J. Maurer — University of Warwick, Coventry, UK

Experiments on hydrogen atom scattering from Ge(111) show bimodal energy loss distributions with two peaks. The first peak corresponds to low energy loss and can be quantitatively reproduced with classical molecular dynamics (MD) simulations. The second peak lies at energy losses equivalent to or above the band gap of Ge and arises from electronic transitions between the valence band and the conduction band. Here, we develop a simple and interpretable model for H/Ge(111) scattering to inform the development of new mixed quantum-classical dynamics simulation methods suitable for the description of such nonadiabatic effects in gas-surface scattering. Using density functional theory data and experimental quantities, we parametrize an effective one-dimensional analytical model based on the Newns-Anderson Hamiltonian. The model allows us to study the coupled electron-nuclear dynamics and their conjugate energy transfer using nonadiabatic molecular dynamics methods such as independent electron surface hopping (IESH), molecular dynamics with electronic friction (MDEF), and the Ehrenfest method. In particular, IESH dynamics qualitatively reproduce the nonadiabatic energy transfer channel observed in the experiment.

O 42.2 Tue 14:15 H11

**Shaping Polarons in Hematite $Fe_2O_3$: From Creation to Charge Dynamics** — •Sreehari Sreekumar[1], Llorenc Albons Caldentey[1], Jesus Redondo Redondo[1], Aji Alexander[1], Sarah Tobisch[2], Michele Riva[2], and Martin Setvin[1] — [1]Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [2]Institute of Applied Physics, Vienna University of Technology, Austria

The non-contact Atomic Force Microscopy (nc-AFM) technique has enabled breakthroughs in single-electron charge manipulation [1]. Here we use this capability to study polaron dynamics. Polarons are self-localized electrons or holes in ionic lattices that are crucial to material properties like conductivity, catalysis, and exotic phenomena such as high-temperature superconductivity and colossal magnetoresistance [2]. Polarons are studied in hematite at the single quasiparticle limit, focusing on the fundamental mechanisms involved in their injection, formation, migration, and interaction with defects [3].

1. Gross, L., et al., Science, 2009. 324(5933).
2. Franchini, C., et al., Nature Reviews Materials, 2021. 6(7).
3. Redondo, J., et al., Science Advances, 2024. 10(44).

The work was supported by project MSMT LL2324 *PoTr*

O 42.3 Tue 14:30 H11

**Observing the directed motion of a single molecule after dissociation on a surface** — •Ilias Gazizullin[1], Matthew Timm[1], Matthias Krinninger[2], Friedrich Esch[2], and Leonhard Grill[1] — [1]Physical Chemistry Department, University of Graz, Austria — [2]Faculty of Chemistry, TU München, Germany

Unidirectional motion of single molecules on surface can be achieved via a rare interplay between the surface and the intramolecular chemical reaction [1]. An alternative approach to achieve controllable molecular motion on surface is to induce dissociation of a molecule, resulting in the recoiling motion of the products [2, 3].

Here, we show how orientation of functional groups of an adsorbed molecule can steer its motion after controlled dissociation of these groups. We study single organic molecules with azido groups adsorbed on Au(111) surface by low temperature scanning tunneling microscopy (STM). The azido group of the adsorbed molecule can be oriented in two possible directions. We applied voltage pulses from the STM tip onto the azido group to induce its dissociation and found that the molecule rotates after dissociation in a specific direction. This directionality clearly depends on the initial orientation of the dissociating azido group, opening new possibilities to induce controlled motion of single molecules on surfaces.

[1] Simpson et al., Nature, 621, 82-87 (2023)
[2] Anggara et al., Sci. Adv., 4 (2018)
[3] Anggara et al., J. Am. Chem. Soc., 138, 7377-7385 (2016)

O 42.4 Tue 14:45 H11

**Nonadiabatic quantum dynamics of molecules scattering from metal surfaces** — •Riley Preston[1], Yaling Ke[2], Samuel Rudge[1], Nils Hertl[3], Raffaele Borrelli[4], Reinhard Maurer[3], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg — [2]Department of Chemistry and Applied Biosciences, ETH Zürich — [3]Department of Chemistry and Department of Physics, University of Warwick — [4]DISAFA, University of Torino

Nonadiabatic coupling between electrons and molecular motion at metal surfaces can strongly impact the dynamics of a scattering molecule [1]. We present a theoretical approach based on hierarchical equations of motion (HEOM) [2], which models the scattering of molecules from metal surfaces and incorporates all nonadiabatic and quantum nuclear effects due to the coupling of the molecular degrees of freedom to the electrons in the metal. The approach is exemplified by its application to NO scattering from Au(111), where we observe multi-quantum relaxation of the bond vibrational state due to coupling to electron hole pairs in the surface, in accordance with experiment. The data obtained by the HEOM approach is also used as a rigorous benchmark to assess various mixed quantum-classical methods, from which we derive insights into the validity range of each method [3].

[1] A. M. Wodtke, Chem. Soc. Rev. 45, 3641-3657 (2016).
[2] Y. Ke, R. Borrelli, and M. Thoss, J. Chem. Phys. 156, 194102 (2022).
[3] R. J. Preston, Y. Ke, S. L. Rudge, N. Hertl, R. Borrelli, R. J. Maurer, and M. Thoss, arXiv preprint arXiv:2410.05142 (2024).

O 42.5 Tue 15:00 H11

**Nonthermal phonon distributions induced by hot electrons** — •Tobias Held, Christopher Seibel, Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau

When an ultrashort laser pulse irradiates a metal, the electrons initially absorb the energy and rapidly establish a hot Fermi distribution. Subsequently, on a picosecond timescale, the electrons transfer energy to the phonon system. Electrons exhibit a stronger coupling to high-wavenumber phonons, leading to nonthermal phonon distributions induced by electron-phonon scattering.

In this study, we use the Boltzmann equation to examine the formation and subsequent relaxation of nonequilibrium phonon distributions. For our model system, we find that the majority of the energy is transferred within 10 ps, while a pronounced phonon nonequilibrium is induced. We observe "hot phonons" at the edge of the Brillouin zone, leading to a collapse of the electron-phonon energy transfer rate. Consequently, a finite temperature difference between electrons and phonons may persist significantly longer than the widely used two-temperature model would predict.

O 42.6 Tue 15:15 H11

**Electronic friction simulations of laser-driven hydrogen evolution from copper. Just thermal desorption in a hurry?** — •Alexander Spears, Wojciech G Stark, and Reinhard J. Maurer — University of Warwick, Coventry, UK

Ultrafast light pulses can induce energy transfer between light, electrons, and phonons at interfaces, leading to ultrafast dynamics such as light-driven hydrogen evolution from metal surfaces. Whether this energy transfer can drive photocatalysis through selective energy transfer into certain degrees of freedom remains an open question. Molecular dynamics simulations with electronic friction (MDEF) offer a quantum-classical description of electron-phonon coupling and have previously been used to model ultrafast surface dynamics. However, the effect of different electronic friction approximations on the final energy distributions has not been thoroughly investigated. We present MDEF simulations of light-driven hydrogen evolution from different copper surface facets, enabled by machine-learning surrogate models. For various laser fluences, we study desorption probabilities and final state distributions of desorbed molecules. Our results reveal that the choice of electronic friction approximation significantly affects desorption probabilities. However, the magnitude and nature of friction do not seem to affect the final vibrational, rotational, and translational energy distribution of molecular adsorbates. Within the electronic friction approximation, only the shape of the energy landscape determines these properties and no selective energy transfer occurs. This suggests that thermal and laser-driven desorption may yield similar outcomes.

## O 43: Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale II

Time: Tuesday 14:00–15:45 Location: H24

O 43.1 Tue 14:00 H24

**Kinetics of nucleation and crystallization of sodium chloride based on frozen solution sample preparation apparatus** — •Xinmeng Liu[1], Jiadong Guo[1], Yunzhe Jia[2], Sheng Meng[2], Enge Wang[1], and Ying Jiang[1] — [1]International Center for Quantum Materials, School of Physics, Peking University, Beijing, People's Republic of China — [2]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing, People's Republic of China

Solution environment is ubiquitous and plays a vital role in various fields, especially in the nucleation and crystallization process. Here, we designed and built a new frozen solution sample preparation apparatus compatible with UHV environment, allowing atomic-scale SPM experiments. By utilization of this apparatus, we successfully transferred NaCl solution in glassy states onto the Au(111) substrate. The qPlus-based AFM with CO tip characterized the kinetics of ions nucleation and crystallization after annealing. We found that the ions tend to form disordered networks with water molecules at the initial stage of nucleation, and then adjust to ordered crystals. Furthermore, ions continue to crystallize on the formed island surface by way of chain growth. This is different from the previous view that NaCl nucleation follows the classical nucleation theory. In addition, we also captured the existence of a small crystal nucleus composed of several ions, which is surrounded by water molecules that help the nucleus to further grow. Our results provide new insights into solution process and will have significant effect on the mechanism of material synthesis.

O 43.2 Tue 14:15 H24

**Wavefunction Reconstruction of Excitonic Edge States using Machine Learning** — •Aritra Mishra, Sidhartha Nayak, and Alexander Eisfeld — Max Planck Institute for the Physics of Complex Systems

A typical problem in quantum mechanics is to reconstruct the eigenstate wave functions from measured data. In the case of molecular aggregates, the information about the excitonic eigenstates is important to understand the optical and transport properties [1]. The reconstruction of the wavefunction coefficients from the near field absorption spectra is shown for a linear and a 2D molecular arrangement [2].

Here, we consider the aggregates arranged in two sublattices in a 2D arrangement, each sublattice having a particular orientation of the molecular transition dipole moment, that shows topological edge states as described in [3]. We show the reconstruction of the excitonic wave function for $N = 50$ molecules and move to $N = 200$, in the presence of disorder in the molecular dipole orientations and noise in the spectra. We observe a better reconstruction for higher noises considering all the input spectra for the electric field polarisation of the nanotip along the $x$, $y$ and $z$ axes.

[1] X. Gao and A. Eisfeld, J. Phys. Chem. Lett. 9, 6003 (2018)
[2] F. Zheng, X. Gao and A. Eisfeld, Phys. Rev. Lett. 123, 163202 (2019)
[3] J. Yuen-Zhou, S. K. Saikin, N. Y. Yao and A. Aspuru-Guzik, Nature Materials 13, 1026 (2014)

O 43.3 Tue 14:30 H24

**Probing topological Floquet states in graphene with ultrafast STM** — •Nils Jacobsen[1,2], Melanie Müller[3], Michael Schüler[4,5], Martin Wolf[3], Angel Rubio[2,6], and Michael Sentef[1,2] — [1]ITP, University of Bremen, Bremen, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Fritz Haber Institute, Berlin, Germany — [4]Laboratory for Materials Simulations, Paul Scherrer Institut, Villigen, Switzerland — [5]Department of Physics, University of Fribourg, Fribourg, Switzerland — [6]Center for Computational Quantum Physics The Flatiron Institute, New York, USA

Floquet band engineering enables the control of solids via periodic laser driving. The light-induced quantum anomalous Hall effect (QAHE) in graphene with circularly polarized light [1] has been measured in ultrafast transport [2] and recently, Floquet replica bands under linearly polarized light have been reported in time-resolved photoemission spectroscopy [3]. Here, we explore the possibility of probing (topological) Floquet states in graphene with ultrafast scanning tunneling microscopy (USTM) as a complementary experimental technique [4]. Being highly sensitive to gap openings in the local density of states and the formation of edge states, USTM is a promising and versatile tool for probing light-induced topological states in quantum materials.

[1] Oka et al. PRB 79, 081406(R) (2009) [2] McIver et al. Nat. Phys. 16, 38-41 (2020) [3] Merboldt et al. arXiv:2404.12791 (2024) , Choi et al. arXiv:2404:14392 (2024) [4] Müller Prog. Surf Sci. 99, 100727 (2024)

O 43.4 Tue 14:45 H24

**Theoretical Study of Electronic and Optical Properties in Edge-Modified Graphene Nanoribbons** — •Jian Cheng Wong[1], Song Jiang[2], Sofia Canola[1], Alex Boeglin[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, IPCMS, CNRS, UMR 7504, F-67000 Strasbourg, France

Graphene nanoribbon (GNR) exhibits electronic and optical properties tunable by its geometry. One such approach is to introduce localized electronic states by modifying the edge structure. A previous study [1] using scanning tunneling microscopy-induced luminescence (STML) revealed that the presence of localized single-particle end states in GNR contributed to the formation of localized optical excitations. Here we provide an extensive theoretical description of such excitations on the modified edge structure of GNRs, and how it interacts with the end states. To that end, we develop a many body model that incorporates ab initio electronic structure methods and elucidate the sequence of events involved that leads to the eventual light emission under STML. From this model, we compare the electroluminescence maps obtained with experimental results and show the microscopic details of the localized states probed by STML.

[1] Song et al., Science, 379(6636), 1049-1054 (2023).

O 43.5 Tue 15:00 H24

**Correlations between noise and electroluminescence in graphene nanojunctions** — •Sascha Korn, Michael Krieger, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg

Light emission in scanning tunneling microscopy is often explained by the granularity of charge and should be therefore correlated with shot noise. Also, hot electrons may create both noise and thermal luminescence [1,2]. Using planar graphene nanojunctions, we study the phenomenon of electroluminescence in the point contact regime in a simple and well controlled electromagnetic environment. A spectral analysis of such measurements perfectly follows Planck‘s law and unambiguously supports the thermal picture. We present experimental data that correlate electrical noise measurements and optical spectroscopy, providing an in-depth view into the microscopic processes.

[1] Ott, C., Götzinger, S. & Weber, H. B. Thermal origin of light emission in nonresonant and resonant nanojunctions. Phys. Rev. Res.

2, 042019 (2020)

[2] Korn, S., Popp, M.A. & Weber, H.B. A point-like thermal light source as a probe for sensing light-matter interaction. Sci Rep 12, 4881 (2022)

O 43.6 Tue 15:15 H24

**Photon blockade in current-driven single-molecule emitters** — Andrés Bejarano[1,2], •Moritz Frankerl[1], Rémi Avriller[2], Fabio Pistolesi[2], and Thomas Frederiksen[1,3] — [1]Donostia International Physics Center, Spain — [2]Univ. Bordeaux, CNRS, LOMA, France — [3]Ikerbasque, Bilbao, Spain

We consider photon emission from a single electronic level embedded in a strongly damped cavity, where photon emission is driven by electronic tunneling events. Using a Lindblad master equation approach we investigate the system dynamics, photon emission spectrum as well as the second-order coherence function $g^{(2)}(\tau)$ [1]. We demonstrate that many features observed in scanning tunneling microscopy light-emission experiments can be explained with this simple model. Specifically, restricting the applied bias to the first emission threshold, we find antibunching in the photon statistics irrespective of the coupling strength to the cavity [2]. Employing a higher bias leads to a excitation of states with a photon number greater than one and thus the system shows bunching behavior as well as an emergence of two distinct time scales in the dynamics of $g^{(2)}(\tau)$. [1] Q. Schaeverbeke, R. Avriller, T. Frederiksen, F. Pistolesi, PRL 123, 246601 (2019) [2] P.Merino, C. Große, A. Roslawska, K. Kuhnke, K. Kern, Nat. Comm. 6, 8461 (2015)

O 43.7 Tue 15:30 H24

**Attosecond charge transfer in atomic-resolution scanning tunnelling microscopy** — •Katharina Glöckl[1], Simon Maier[1], Raffael Spachtholz[1], Carlos Bustamante[2], Korbinian Pürckhauer[1], Franz J. Giessibl[1], Franco Bonafé[2], Markus A. Huber[1], Angel Rubio[2], Jascha Repp[1], and Rupert Huber[1] — [1]Department of Physics & Regensburg Center for Ultrafast Nanoscopy (RUN), Universität Regensburg — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg

Scanning tunnelling microscopy (STM) driven with single-cycle terahertz pulses has afforded atomic-scale slow motion videos of single molecular orbitals. Driving tunnel currents with the carrier field of near-infrared light could improve the temporal resolution from ~100 fs down to attoseconds. Yet, competing multi-photon processes and thermal effects pose severe challenges in this spectral domain.

Here, we introduce an attosecond STM concept that is largely immune against thermal artifacts. By pulse synthesis, we periodically vary the waveform of single-cycle near-infrared pulses to drive tunnelling currents while keeping the thermal load on the tip constant. In a non-degenerate pump-probe scheme, we observe clear attosecond features in the sub-cycle currents and demonstrate atomic resolution by taking snapshot images of a single Cu adatom on a silver surface. Our results pave the way to recording the fastest relevant dynamics of electrons within atoms, molecules and quantum materials in actual attosecond atomic videography.

## O 44: Poster Oxides and Insulator Surfaces: Structure, Epitaxy and Growth

Time: Tuesday 18:00–20:00 Location: P2

O 44.1 Tue 18:00 P2

**The dynamic interaction of size-selected Pt clusters with $CeO_2$/Rh(111)** — •Mina Soltanmohammadi, Johanna Reich, Barbara A.J. Lechner, and Friedrich Esch — Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, Germany

Recent studies on Pt clusters supported on ceria have revealed interesting cluster formation and redispersion processes that can be induced by cyclic redox treatments [1]. These catalysts' activity for combustion is linked to the verge of cluster formation. Here, we investigate the dynamic interaction of size-selected Pt clusters with $CeO_2$(111) thin films at the atomic scale, using a combination of scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). We present a preparation protocol to obtain highly clean, crystalline and stochiometric $CeO_2$(111) thin films with extended terraces and well-defined monoatomic steps. Distinct oxygen vacancy distributions are obtained by either annealing in vacuum or reducing in a methanol atmosphere. We then systematically explore the interaction of Pt clusters with the support, particularly the mobility and sintering in dependence of the defect state. The influence of support stoichiometry and the parameters controlling the resulting cluster dispersion are presented. Finally, we present first studies of the Pt dispersion under cyclic oxidizing ($O_2$) and reducing (methanol) conditions at elevated temperatures, focusing on the resulting cluster configurations at the atomic scale.

[1] Farnesi Camellone et al., ACS Catal. 2022, 4859.

O 44.2 Tue 18:00 P2

**Search for crystalline $SiO_2$ on the wet chemically treated 6H-SiC(0001) surface** — •Paul Schöngrundner[1], Igor Sokolovic[2], and Ulrike Diebold[2] — [1]Department of Physical Chemistry, University of Graz, 8010, Austria — [2]Department of Applied Physics, Technical University of Vienna, 1040, Austria

A 6H-SiC(0001) surface was found to host a crystalline superstructure consisting of $SiO_2$ after wet chemical treatment. This surface was envisioned as a model system for surface chemistry studies. In order to replicate and optimize this film, chemical and thermal treatments were investigated systematically. Using atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED), an improved cleaning methodology was established, resulting in contaminant-free surfaces (except adventitious C), but they were terminated with amorphous $SiO_2$ instead of a crystalline film. If the sample was treated by repeating the original cleaning technique, which was finished with Extran and milliQ sonication, without subsequent boiling in $H_2O$, the original surface termination could be re-prepared. However, this was accompanied by P and Cr contamination. It is hypothesized that P and/or Cr contamination were ultimately responsible for the crystalline silicon oxide overlayer.

O 44.3 Tue 18:00 P2

**Pulsed laser deposition of epitaxial hematite $\alpha$-$Fe_2O_3$ thin films on $Al_2O_3(1\bar{1}02)$** — •Sarah Tobisch, Giada Franceschi, Michael Schmid, Gareth Parkinson, Ulrike Diebold, and Michele Riva — Institute of Applied Physics, TU Wien, Vienna, Austria

Hematite $\alpha$-$Fe_2O_3$ is a widely used support material for catalysis due to its abundance and high stability at ambient pressures. However, the insulating nature of the material poses major challenges, as it makes it difficult to achieve sufficient conductivity for techniques such as scanning tunnelling microscopy (STM). Samples commonly consist of natural crystals that can contain a variety of impurities as well as structural defects. The former problem is hardly controllable while the latter can lead to mechanical instabilities. While the conductivity can be improved by growing Ti-doped epitaxial films, the synthesis of hematite single crystals is still in its infancy and the size of these crystals is insufficient for many surface-analysis techniques. Therefore, new strategies to ensure the growth of flat and atomically defined doped films without the need of natural-crystal substrates are highly desired.

In this work, epitaxial growth of Ti-doped $Fe_2O_3$ on $Al_2O_3(1\bar{1}02)$ was investigated using a pulsed-laser-deposition (PLD) system with high-pressure reflection high-energy electron diffraction (RHEED) to optimize the growth conditions and monitor the growth behavior. The morphology and composition of the film's surface was characterized using x-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and STM.

# O 45: Poster Spins on Surfaces at the Atomic Scale

Time: Tuesday 18:00–20:00 Location: P2

O 45.1 Tue 18:00 P2

**Scanning Tunneling Microscopy and Spectroscopy of YbPc2 Molecules** — •Jonas Arnold[1], Kwan Ho Au-Yeung[1], Wantong Huang[1], Paul Greule[1], Christoph Sürgers[1], Wofgang 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-phythalocyanine complexes [1]. In this investigation, YbPc2 molecules are studied using scanning tunneling microscopy (STM) and spectroscopy (STS) to identify potential indicators of a magnetic signature. In the gas phase, the YbPc2 molecule is expected to exhibit a radical spin localized at its ligands as well as an f-shell electron spin $S = 1/2$ and 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 YbPc2 on Ag(100) that reveal distinct orbital features which vary for the first, second and third molecular layer. Similarly, the orbital signatures change when introducing a thin dielectric decoupling layer of MgO between the molecule islands and the electron bath. We discuss these results in the context of charge transfer between the molecular film and the underlying substrate [2]. [1] Wernsdorfer, W. et al., Advanced Materials 31, 1806687 (2019). [2] Hollerer, M. et al., ACS nano 11, 6252-6260 (2017).

O 45.2 Tue 18:00 P2

**Magnetic adatom manipulation on monolayer transition metal dichalcogenides** — •Daniel Jansen[1], Katharina Offermann[1], Tfyeche Tounsi[1], Affan Safeer[1], Jeison Fischer[1], Arkady Krasheninnikov[2], Nicolae Atodiresei[3], Thomas Michely[1], Hannu-Pekka Komsa[4], and Wouter Jolie[1] — [1]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [2]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Jülich, Germany — [4]Faculty of Information Technology and Electrical Engineering, University of Oulu, Oulu, Finland

Two-dimensional materials are found to host a large variety of correlated phases. A promising approach towards understanding and controlling these phases is by means of atomic manipulation.

Here we compare two systems for atomic manipulation experiments: Fe on 1H-MoS$_2$ and Fe on 1H-TaS$_2$. We find that manipulation of Fe on 1H-MoS$_2$ results in point defects (sulfur vacancies) [1], which we investigate using scanning tunneling microscopy and spectroscopy. In contrast, we find that single Fe adatoms can be laterally moved on 1H-TaS$_2$, enabling construction of lattices consisting of tens of adatoms. We additionally report on the observation of two inequivalent adsorption sites for Fe, hollow and Ta-top sites, which manifest as differences in the adatom's apparent height.

[1] Jansen et al., Phys. Rev. B, **109**, 195430, 2024

O 45.3 Tue 18:00 P2

**investigating the origins of spin-polarization in Au(111) : experiments vs theory** — •Sourour Ayari[1], Laurent Nicolaï[1], Aki pulkkinen[1], Ridha Eddhib[1], Saleem Khan[1], Trung Phuc[1], Ján Minár[1], and Mauro Fanciulli[2,3] — [1]New Technologies - Research Centre, University of West Bohemia, 301 00 Pilsen, Czech Republic. — [2]CY Cergy Paris University, France — [3]CEA Paris Saclay, France

This study explores the origins of spin polarization in semi-infinite Au(111), examining whether the observed spin polarization arises primarily from the system's initial states or solely through the Photoemission process. To address this, we will integrate both experimental and theoretical results to provide an understanding of this spin-polarization origins, we calculate the electronic band structure with and without the influence of Mott-Scattering, while isolating additional factors, such as the Rashba effect[1]. On the theoretical side the calculations are performed using the SPRKKR method [2,3] which is based on DFT calculations, which will account for fundamental effects, while the additional one-step model will account for the photoemission process.

[1]E. E. Krasovskii and E. V. Chulkov Phys. Rev. B 83, 155401 (2011) [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011) [3] J. Braun et al., Phys. Rev. B 88, 205409 (2013)

O 45.4 Tue 18:00 P2

**Coherent driving of interacting spins in single molecules** — •Maria Steiner and Andrea Donarini — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

The low energy spectrum of neutral closed shell molecules generically exhibits a set of singlet and triplet excited levels. The latter arises due to the exchange interaction between the unpaired electrons in singly occupied frontier orbitals. Moreover, the spatial anisotropy of these molecular states, combined with the spin-dipolar interaction, induces a zero-field splitting of the triplet. In recent AFM-ESR experiments on pentacene [1] Rabi oscillations between two of the split triplet states have been demonstrated. We now extend this concept to the full triplet space. By means of multiple frequency coherent driving, we investigate theoretically the rich dynamics of this molecular qutrit in search, for example, of the analogue of the dark states observed for $\Lambda$-systems in atomic physics.

[1] Sellies et al., Nature **624**, 64-68 (2023).

O 45.5 Tue 18:00 P2

**A molecular spin on a scanning probe tip enables quantum sensing at the atomic scale** — Taner Esat[1,2], Dmitriy Borodin[3,4], •Jeongmin Oh[1,2], Andreas Heinrich[3,4], Stefan Tautz[1,2,5], Yujeong Bae[3,4], and Ruslan Temirov[1,2,6] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich; Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology; Jülich, Germany — [3]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS); Seoul, South Korea — [4]Department of Physics, Ewha Womans University; Seoul, South Korea — [5]Experimentalphysik IV A, RWTH Aachen University; Aachen, Germany — [6]Faculty of Mathematics and Natural Sciences, Institute of Physics II, University of Cologne; Cologne, Germany

In this work, we fabricate a single-molecule quantum sensor on a scanning tunneling microscope (STM) tip by attaching Fe atoms and a PTCDA (3,4,9,10-perylenetetracarboxylic-dianhydride) molecule to the tip apex. The PTCDA molecule is a spin-1/2 system on the STM tip and serves as a two-level quantum system in a magnetic field. We probe this molecular spin system by electron spin resonance and achieve about 100 neV resolution in energy. The functionality of the quantum sensor we demonstrate by measuring the magnetic and electric dipole fields emanating from a single Fe atom and an Ag dimer on an Ag(111) surface with sub-angstrom spatial resolution [T. Esat, D. Borodin, J. Oh et al. Nat. Nanotechnol. 19, 1466 (2024)].

O 45.6 Tue 18:00 P2

**Thermometry of a millikelvin scanning probe junction with spin-flip inelastic electron tunnelling spectroscopy** — •Emilio Scontrino[1,3], Stefan Schulte[2,3], Taner Esat[3], Markus Ternes[1,3], Stefan Tautz[1,3], and Ruslan Temirov[2,3] — [1]RWTH Aachen — [2]Universität zu Köln — [3]Forschungszentrum Jülich, PGI-3, Germany

Organic molecules attached to the apex of a scanning probe tip have recently emerged as promising sensors for electric and magnetic fields at atomic scales [1, 2, 3]. Here, we functionalize the tip of a millikelvin scanning tunnelling microscope (STM) [4] with a 1,4,5,8-naphthalene tetracarboxylic dianhydride (NTCDA) molecule. We measure the inelastic spin-flip excitations of this molecular spin 1/2 system in an out-of-plane magnetic field of 7 T varying the temperature of the adiabatic demagnetization cryostat between 30 mK and 1.2 K. To perform thermometry of the STM junction we fit the temperature-dependent smearing of the spin-flip excitation spectra using the third-order perturbation theory in the Appelbaum-Anderson-Kondo framework [5].

[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. Nano. 19, 1466 (2024) [4] T. Esat et al., Rev. of Sci. Instr. 92 (6) (2021) [5]

M. Ternes, New J. Phys. 17, 063016 (2015)

O 45.7 Tue 18:00 P2

**Investigation of the Kondo effect in complex, artificially built, single molecule structures** — •Lars Pütz[1], Daria Sostina[1], Taner Esat[1,2], Stefan Tautz[1,2,3], Ruslan Temirov[1,4], and Markus Ternes[1,2,5] — [1]Peter-Grünberg-Institute for Quantum Nanoscience, Research Center Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, 52425 Jülich, Germany — [3]Institute of Physics IV, RWTH Aachen University, 52074 Aachen, Germany — [4]Institute of Physics II, University of Cologne, 50937 Cologne, Germany — [5]Institute of Physics IIB, RWTH Aachen University, 52074 Aachen, Germany

In engineered spin systems, strongly correlated many-body phenomena such as nontrivial topology, Kondo screening and highly correlated long-range states can be constructed and studied by site-selective measurements with scanning tunneling microscope (STM) tips [C. Zhao et al., Nat. Nanotech. 2024]. Here we show how many-body phenomena evolve by controlled manipulation of NTCDA molecules on Ag(111) using the tip of an STM. Building small clusters of 2-5 molecules and tuning their spatial geometry reveals complexly patterned Kondo resonances and, in addition, an electric field-dependent strong increase in conductance, which we attribute to the collapse of Kondo correlations [S. Arabi et al., arXiv 2022]. Single NTCDA molecules on the other hand show no detectable spin signature, despite the clear formation of Kondo resonances in clusters where their high symmetry with respect to the surface is broken.

O 45.8 Tue 18:00 P2

**Investigation of the Yu-Shiba-Rusinov states arising from single Fe atoms on superconducting $2H$-NbS$_2$** — •Margarete Huisinga, Werner M.J. van Weerdenburg, Lisa M. Rütten, and Katharina J. Franke — FachbereichPhysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Magnetic adatoms on a superconductor give rise to states within the superconducting gap due to the interaction of the unpaired spin(s) with the Cooper pairs of the substrate. These so-called Yu-Shiba-Rusinov (YSR) states are therefore isolated from the rest of the electronic structure of the system, which makes them interesting building blocks for artificial molecules or the design of band structures, if the YSR states of multiple atoms hybridize. The YSR states are especially long range on 2D materials, which enables hybridization over a large spacing. Previous experiments on the hybridization of YSR states performed on NbSe$_2$ were limited by a charge density wave [1], which is not present in $2H$-NbS$_2$.

Using scanning tunneling microscopy and spectroscopy, we investigate single Fe atoms on superconducting $2H$-NbS$_2$. We find that Fe adsorbs in two different adsorption sites on the substrate, each with a distinct set of YSR states. We map the spatial distribution of these YSR states to determine their symmetry and find long-ranged YSR features extending up to 4 nm. Additionally, we observe a tip-induced shift in the energy of the YSR states for one adsorption site species.

[1] Liebhaber et al. Nat Commun 13, 2160 (2022).

O 45.9 Tue 18:00 P2

**Hybridization of Yu-Shiba-Rusinov states in magnetic clusters on Pb(111)** — •Katharina Biel, Bharti Mahendru, Werner M. J. van Weerdenburg, Lisa M. Rütten, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The unpaired spin of a magnetic impurity on a superconducting substrate interacts with the Cooper pairs via potential and exchange scattering. This leads to local in-gap bound states, so-called Yu-Shiba-Rusinov (YSR) states. The hybridization of close-by atoms can be described by linear combinations of the YSR states [1,2].

We investigated self-assembled manganese (Mn) and iron (Fe) clusters on superconducting lead (Pb(111)) by scanning tunneling microscopy and spectroscopy. While the topography essentially shows featureless protrusions, the differential conductance maps reflect characteristic shapes of the YSR states. We employ a phenomenological hybridization model [3] to simulate the observed shapes. In particular, we show atomic configurations which lead to chiral YSR patterns.

[1] Ruby, M., et al., PRL 120, 156803 (2018); [2] Amann, S., et al., PRB 108, 195403 (2023); [3] Rütten, L., et al., ACS Nano 18, 30798 (2024)

O 45.10 Tue 18:00 P2

**Investigation of impurity states on the high-temperature superconductor Bi$_2$Sr$_2$Ca$_1$Cu$_2$O$_{8+x}$ via scanning tunneling microscopy** — •Melvin Grumser, Verena Caspari, Werner M. J. van Weerdenburg, and Katharina J. Franke — Freie Universität Berlin, Department of Physics, Arnimallee 14,14195 Berlin, Germany

The interaction of magnetic impurities and superconductors gives rise to impurity states in the superconducting gap, which have been widely studied for s-wave superconductors [1]. For d-wave superconductors however, only few experiments addressing the interplay of local spins and Cooper pairs, governed by an anisotropic order parameter and non-vanishing density of states (DOS) in the superconducting gap have been reported [2,3].

Here, we investigated the interaction between the high-temperature d-wave superconductor Bi$_2$Sr$_2$Ca$_1$Cu$_2$O$_{8+x}$ and magnetic adatoms on the atomic scale using scanning tunneling microscopy. We present measurements conducted on scandium, iron and manganese adatoms, expected to display different amounts of in-gap states due to the different number of unpaired electrons. We find strong variations in the spectra that we ascribe to different adsorption sites and variations of the density of states across the substrate.

[1] W. Heinrich, I. Pascual, K. J. Franke, Progress in Surface Science 93 (2018)

[2]U. Erdenemunkh, M. C. Boyer, Physical review letters 117 (2016)

[3] J. Davis, Nature 411 (2001)

O 45.11 Tue 18:00 P2

**Atomic-scale Josephson spectroscopy performed over magnetic clusters on Pb(111)** — •Bharti Mahendru[1], Martina Trahms[1,2], Katharina Biel[1], Werner M. J. van Weerdenburg[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Université Grenoble Alpes, CNRS, Institut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

When two superconducting leads are brought in close proximity, they form a Josephson junction (JJ). In a JJ, quantum tunnelling of Cooper pairs occurs without an applied voltage between the two superconductors with a phase difference. To study the properties of Cooper-pair tunneling at the atomic scale, a scanning tunneling microscope is a powerful tool. A JJ forms by approaching the tip to the sample. Previously, it has been shown that a Josephson junction including a single magnetic adatom shows non-reciprocity in the retrapping current [1]. This expression of the Josephson-diode effect was ascribed to the broken particle-hole symmetry induced by the Yu-Shiba-Rusinov (YSR) states inside the superconducting energy gap. Here, we investigate the effect of hybridized YSR states of self-assembled Fe clusters on Pb(111). We find non-reciprocal retrapping currents that we correlate with the asymmetry in the YSR states and their spatial distribution.
[1] Martina Trahms et al., *Nature* 615, (2023)

O 45.12 Tue 18:00 P2

**Driving nuclear spin transitions on a single atom using ESR-STM** — •Hester Vennema, Cristina Mier Gonzalez, Evert Stolte, Rik Broekhoven, Jinwon Lee, and Sander Otte — Delft University of Technology, The Netherlands

The spin of a single nucleus is a prime candidate for quantum information applications due to its weak coupling to the environment and subsequently longer coherence times [1]. Using the high energy resolution of electron spin resonance (ESR) in combination with the high spatial resolution of scanning tunneling microscopy (STM), it is possible to measure the hyperfine interaction between the nucleus and an electron for single atoms on a surface [2].

A recent effort has successfully resolved the coherent dynamics of a hyperfine-driven interaction between nuclear and electron spin [3]. Moreover, the lifetime of the nuclear spin has been measured to be in the order of seconds [4].

In this study we use a double resonance measurement scheme to resolve nuclear spin transitions of a single 47Ti isotope with a spin of I=5/2. Additionally, we are able to selectively drive multiple transitions directly.

[1] Pla et al. (2013), Nature 496, 334-338

[2] Willke et al. (2018), Science 362, 336-339

[3] Veldman et al. (2024), Nat. Comm. 15, 7951

[4] E. Stolte et al. (2024), arXiv:2410.0870

O 45.13 Tue 18:00 P2

**Nanoscale Control of Quantum States in Radical Molecules**

**on Superconducting Pb(111)** — •Chao Li, Jung-Ching Liu, Outhmane Chahib, Thilo Glatzel, Rémy Pawlak, and Ernst Meyer — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland.

Superconducting surfaces hosting magnetic impurities provide a promising framework for applications in quantum technology. Here, we demonstrate the manipulation of magnetic states in the radical molecule 4,5,9,10-tetrabromo-1,3,6,8-tetraazapyrene (TBTAP) deposited on a Pb(111) superconducting surface, utilizing low-temperature scanning tunneling microscopy. Tunneling spectroscopy reveals the presence of Yu-Shiba-Rusinov (YSR) states near the Fermi level for isolated TBTAP molecules. By varying the tip-molecule distance, we induce a quantum phase transition between singlet and doublet ground states. Furthermore, introducing a second TBTAP molecule enables tuning of the YSR state position through modifications in relative distance and orientation, with specific configurations leading to the splitting of YSR states. Extended molecular chains, up to pentamers, exhibit periodic patterns of charged and neutral molecules, where even-numbered chains form a distinct charged dimer structure at one terminus. This dimer position can be manipulated, allowing for information encoding within the chain.

O 45.14 Tue 18:00 P2

**Exchange interactions of spin states in coupled triangular nanographenes** — •Suyash Singh[1], Nils Krane[1], Elia Turco[1], Roman Fasel[1,2], and Pascal Ruffieux[1] — [1]Empa - Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf (Switzerland) — [2]Department of Chemistry and Biochemistry, University of Bern, 3012 Bern, Switzerland

Zigzag-edged triangular nanographenes (triangulenes) are promising realizations of spin qubits at a molecular level, with a total spin $S$ scaling with the length of their edges. Chemical design and on-surface synthesis methods allow atomically precise engineering of carbon-based $\pi$–systems with strong spin-spin interactions, using triangulene units as building blocks. Exploiting the rules governing the exchange interactions, functional groups and spacer molecules, such as phenyl rings, can be used to tune the sign and magnitude of the exchange coupling between the triangulene units. We present the bottom-up fabrication of correlated spin platforms using the two smallest members of the triangulene family, the spin S=1/2 phenalenyl and S=1 [3]triangulene. We analyze the origin of spin-polarized states and spin excitations using a tight-binding and mean-field Hubbard Model for the $\pi$–orbital network. With an estimate of the couplings within the spin cluster, we describe it using an effective Heisenberg model. The spin excitations are then investigated experimentally using inelastic electron tunneling spectroscopy. Specifically, we summarize the results on dimers and trimers, where the exchange mechanisms can be investigated systematically by hydrogenation and selective re-activation of single spins.

O 45.15 Tue 18:00 P2

**Properties of magnetic atoms on a hexagonal insulating lattice** — •Johannes Schust, Henrik Lichtl, Julian Zeitler, Lukas Arnhold, Sebastian Loth, and Susanne Baumann — University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany

The symmetry of the immediate surrounding of an atom heavily influences its static properties and also governs its dynamics. For the exploration of atomic-scale systems by scanning tunneling microscopy (STM), the choice of a suitable thin film is thus key. While most preceding works take advantage of two- or four-fold underlying symmetries, we focus on the hexagonal surface of zinc oxide (ZnO) monolayers. Hexagonal substrates bear the potential for exploring spin frustration effects on a surface, realized by the assembly of magnetic nanostructures built atom-by-atom. ZnO, as a wide bandgap semiconductor [1], is employed to mitigate electron scattering between the Ag(111) substrate and the adsorbed species on the sample. We develop a reliable method to prepare the aforementioned substrate and carry out comprehensive characterization of cobalt (Co) and manganese (Mn) atoms in the present environment. These efforts provide the foundation for investigating novel dynamical aspects of frustrated systems on the atomic scale.

[1] A. Shiotari et al. J. Phys. Chem. (2014)

O 45.16 Tue 18:00 P2

**Multiplet calculations of magnetic atoms on a hexagonal insulator** — •Julian Zeitler[1], Johannes Schust[1], Henrik Lichtl[1], Lukas Arnhold[1], Sebastian Loth[1,2], and Susanne Baumann[1] — [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

Novel designs for computational devices may offer improvements in energy efficiency, especially if they include a combination of storing and processing parts in one unit. In such designs, the building blocks should enable slow and fast dynamics, and allow for precise control over the system. Atomic-scale frustrated spin systems combined with atom manipulation capabilities of a scanning tunneling microscope (STM) are a promising prospect in this field. Magnetic atoms placed on a thin hexagonal insulator, such as zinc oxide (ZnO), can potentially be used to realize such systems. As the magnetic atoms interact with their substrate, it is important to understand the substrate's influence on the atoms' characteristics. We use multiplet calculations to study the interactions of individual magnetic atoms with the ZnO substrate. With these calculations, we can make predictions about the magnetic characteristics of different atoms placed on top of this hexagonal substrate, in particular their orbital and spin moments. We are particularly interested in finding atomic-scale systems that, combined with atom manipulation capabilities of an STM, allow for further advancements in the field of atomic-scale frustrated spin systems.

O 45.17 Tue 18:00 P2

**Exploiting YSR States for Driving Spin Transitions in a Magnetic Field** — •Maneesha Ismail[1], Juan Carlos Cuevas[2], and Christian R. Ast[1] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Universidad Autónoma de Madrid, Madrid, Spain

In recent years, advances in the field of atomic scale electron spin resonance (ESR-STM) have made it possible to manipulate single spins and observe their interaction [1,2]. In this work, we exploit the tip confinement of superconductivity in a magnetic field to explore a new candidate system, namely Yu-Shiba-Rusinov states. We present how the Zeeman-split states behave under microwave irradiation. Our theory, which is based on a Green's function approach, corroborates the idea that the presence of the YSR state can be used to detect a change in the spin population. A new sample system could open the path to observing new phenomena in the field of spintronics and quantum computing.

1. K. Yang et al., Science 366 (6464), 509-512
2. L. Sellies et al., Nature 624, 64, 2023.

O 45.18 Tue 18:00 P2

**Tuning the interaction between spin triplet states at the single-molecule level** — Lorenz Meyer, •Maximilian Kögler, Robert Henninger, Nicolas Néel, and Jörg Kröger — Technische Universität Ilmenau, Ilmenau, Germany

In a scanning tunneling microscope junction, two molecular spins - one nickelocene (Nc) decorating the tip and another adsorbed on Pb(111) - are approached toward each other. Simultaneously, inelastic electron tunneling spectra reveal the evolution of spin excitations with increasing magnetic exchange interaction. An avoided energy level crossing occurs at the verge of the Nc-Nc contact. Modeling of the spectra hints at the exchange coupling of tunneling electrons to the Nc spins as the origin. Funding by the DFG through KR 2912/18-1 and KR 2912/21-1 and the BMBF through the ForLab initiative is acknowledged.

# O 46: Poster Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties

Time: Tuesday 18:00–20:00 Location: P2

O 46.1 Tue 18:00 P2

**Electronic Properties of Interfaces between N-Heterotriangulene Donors and Strong Tetracyanoquinodimethane Acceptors** — •Mohsen Ajdari[1], Jakob Roth[1], Ronja Pappenberger[1], Christian Walla[2], Ina Michalsky[3], Friedrich Maass[1], Milan Kivala[3], Andreas Dreuw[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen — [3]Organisch-Chemisches Institut, Heidelberg University

N-Heterotriangulenes (N-HTAs) are promising functional molecules with significant potential for optoelectronic applications, in particular, as electron donors in donor/acceptor (D/A) systems. This study explores the electron-donating properties of two N-HTAs, N-HTA 550 and N-HTA 557, at interfaces with well-known tetracyanoquinodimethane acceptors, TCNQ and F4TCNQ. Using high-resolution electron energy loss spectroscopy (HREELS) combined with quantum chemical calculations, we investigated the electronic properties of D/A interfaces adsorbed on Au(111) [1]. For all D/A combinations, low-energy electronic transitions ($E<2.5$ eV) associated with charge transfer (CT) states are identified. Quantum chemical calculations rule out the formation of ground-state CT complexes. Instead, CT in the excited state, in which an electron-stimulated CT from the N-HTAs to TCNQs is the underlying process, is proposed. The energies of the CT states are determined by the values of the ionization potential and electron affinity of the involved donor and acceptor.
[1] M. Ajdari et al., J. Phys. Chem. C, 128, 14399-14406 (2024)

O 46.2 Tue 18:00 P2

**Self-assembly of magnetic complex on Cu (111) using scanning tunneling spectroscopy: probing Kondo resonance and decomposition effects** — •Behzad Mortezapour[1], Torben Adam[2], Eike Kuhlemann[2], Felix Tuczek[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, Germany

The spin-crossover complex bis-(hydro-tris-(3-methyl-pyrazolyl)-borat)-Iron(II) on Cu (111) at ambient temperature was investigated with a scanning tunneling microscope (STM) under ultrahigh-vacuum conditions at a temperature of 4.6 K. The three-dimensional molecules self-assemble into ordered two dimensional arrays while some decomposition also occurs. The STM images of the intact molecules exhibit a significant dependence on the bias voltage and spectra of the differential conductance (dI/dV) show a zero-bias resonance that we tentatively attribute to the Kondo effect. Time series of the current reveal abrupt transitions that possibly are linked to spin switching. In addition, negative differential resistance is observed from decomposed molecules.

O 46.3 Tue 18:00 P2

**stochastic spin-state switching of a Fe(II) complex on Cu (111)** — •jasmeen jasmeen[1], sujoy karan[1], karl ridier[2], gaël reecht[1], and manuel gruber[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]LCC, CNRS and Université de Toulouse, UPS, INP, 31077 Toulouse, France

Spin-crossover (SCO) molecules exhibit different spin states that make them attractive for nanoscale memory applications. Using scanning tunneling microscopy (STM) at 4.5 K, we studied the [Fe(HB(1,2,4-triazolyl)3)2] complex adsorbed on a Cu (111) surface, focusing on the spin-state switching dynamics. Time traces of the tunneling current revealed switching in the order of milliseconds, which we investigated under a range of bias voltages and currents, providing insights into the stochastic response of this system.

Controlled switching of individual molecules induced by voltage pulses was successful, but also drove a pronounced neighborhood effect: switching a target molecule simultaneously influenced adjacent ones. These events suggest an intermolecular interaction acting on the neighboring molecules due to the conformational changes of the target molecule.

These findings help improving the understanding of electron-induced switching of SCO molecules. Funding from the CRC 1242 is acknowledged.

O 46.4 Tue 18:00 P2

**STM Investigation of Molecular Double Motors** — •Ken Kolar[1], Grant Simpson[1], Ben Feringa[2], and Leonhard Grill[1] — [1]Dept. of Physical Chemistry, University of Graz, Austria — [2]Stratingh Institute for Chemistry, University of Groningen, Netherlands

A molecular motor is a molecule with stator and rotor chemical groups which undergo directional motion relative to each other. They represent potential building blocks for nanoscale machinery and their motion on surfaces is of particular interest. With high-resolution imaging from a scanning tunnelling microscope (STM), we revealed distinct appearances of different conformers of a molecule containing two motor units. Furthermore, motion induced by voltage pulses from the STM tip was studied in detail, investigating unidirectionality. Finally, double motors with additional alkane chains attached to them were deposited, showing distinguishable appearances. The experiments showed that the alkane chain conformation can impact the motion of the molecules.

O 46.5 Tue 18:00 P2

**Excited state alignment of molecular orbitals on the ferroelectric WTe2 bulk crystal** — •Jannis Lessmeister[1], Ralf Hemm[1], Joohyung Park[2], Martin Aeschlimann[1], Oliver L.A. Monti[2], and Benjamin Stadtmüller[3] — [1]Rheinland-Pfälzische technische Universität Kaiserslautern-Landau and Research center OPTIMAS, Kaiserslautern, Germany — [2]University of Arizona, Tucson, USA — [3]Universität Augsburg, Augsburg, Germany

The interaction between organic molecules and ferroelectric domains on WTe$_2$ offers a promising pathway for tuning the electronic properties of hybrid systems. WTe$_2$, a layered transition metal dichalcogenide, exhibits ferroelectricity in its few-layer form due to broken inversion symmetry, resulting in switchable polarization domains. When organic molecules are deposited onto the surface, the local electronic environment created by these ferroelectric domains significantly influences molecular adsorption and electronic coupling.

Utilizing real- and momentum-space photoemission electron microscopy, we investigate how the ferroelectric properties of WTe$_2$ modulate the alignment of excited state energy levels at the FePc/WTe$_2$ interface. Our study elucidates the charge transfer behavior and interaction strength, exploring the role of local electric polarizations for tuning the energy level alignment in molecule-2D material heterostructures.

O 46.6 Tue 18:00 P2

**Momentum space signatures of molecular orbitals on a ferromagnetic surface** — •Martin Anstett[1], Lu Lyu[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The integration of organic molecules with ferromagnetic surfaces is a promising approach to advance spintronic applications. The spin functionalities depend not only on the molecular properties, but also on the energetics and spin polarization of so-called hybrid interface states, which arise due to the hybridization between molecular orbitals and substrate states.

This work focuses on momentum space imaging of the adsorption-induced modification of molecular orbitals on ferromagnetic surfaces at room temperature. This is challenging due to the lack of ordered or aligned molecules on highly reactive magnetic substrates, which is required for momentum space imaging using ARPES. This limitation can be overcome by using ultrathin cobalt films on Au(111) as a ferromagnetic platform. On this surface, we prepare long-range ordered superstructures using iron phthalocyanine molecules. We combine spin- and momentum-resolved photoemission spectroscopy with photoemission orbital tomography to study the characteristic emission pattern of the orbitals of the adsorbed molecules. Our analysis reveals how the molecules arrange on the cobalt surface, producing distinct photoemission signatures associated with individual molecular orbitals.

O 46.7 Tue 18:00 P2

**Thermal-Driven Coordination Effect for Structural and Electronic Tailoring of a Metal-Organic Network** — •Jonas Gödde[1], Lu Lyu[1,2], Benjamin Stadtmüller[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Experimentalphysik II, Institute of Physics, Augsburg University, Universitätsstraße 2, 86159 Augsburg, Germany

Two-dimensional metal-organic porous networks (2D-MOPNs) have emerged as a unique material platform for designing structural tessellations and emergent electronic states on surfaces. The metal centre in a 2D-MOPN plays a vital role in bridging network and substrate. In this study, we investigate the cobalt-coordination effects in cyano-functionalized hexaaza-triphenylene-hexacarbonitrile (HATCN) on Ag(111). Scanning tunnelling microscopy (STM) reveals that HATCN self-assembles into a well-ordered porous network. A partially occupied LUMO state observed by angle-resolved photoemission spectroscopy (ARPES), indicates charge transfer from the substrate to the molecules. After cobalt deposition, the robust equilibrium, between intermolecular and substrate interactions, preserves the porous structure and molecular orbital states of HATCN, while trapping cobalt in the low-potential pores. Upon post-annealing the molecules coordinate with cobalt atoms, inducing a structural transition and creating distinct energy and momentum states. These results provide insights into tailoring 2D-MOPNs for applications in electronics and spintronics.

O 46.8 Tue 18:00 P2

**Spectroscopic study of the interface between organic molecules and platinum telluride thin films** — •Lorenz Klein, Hibiki Orio, Romana Ganser, Muthu P. T. Masilamani, Maximilian Ünzelmann, and Friedrich Reinert — Universität Würzburg, Experimentelle Physik VII & Würzburg-Dresden Cluster of Excellence, Würzburg, Germany

Van der Waals heterostructures of organic molecules and transition metal chalcogenides (TMCs) represent excellent model systems for the study of weak molecule-substrate interactions.

Here, we use two phases of metallic platinum telluride, which both host spin-polarized surface states in their electronic surface band structures. Using those as substrates, we deposit copper phthalocyanine (CuPc) and study the resulting atomic and electronic interface structure by means of x-ray (XPS) and angle-resolved photoemission spectroscopy (ARPES) as well as low-energy electron diffraction (LEED). On that basis, we discuss the differences in surface ordering, work function, and the binding energies of the observed molecular features.

O 46.9 Tue 18:00 P2

**Fluorescence spectroscopy of linear trans-quinacridone (QA) on KCl/Ag(100): The influence of KCl layer thickness** — •Morris E. L. Mühlpointner and Moritz Sokolowski — Clausius-Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany

The organic dye-molecule linear QA has attracted interest as a fluorescent probe molecule in STM luminescence (STM-LE) experiments [1]. We have performed fluorescence spectroscopy of multilayers on the bare Ag(100) surface and highly diluted layers of QA on an epitaxially grown thin KCl film on Ag(100) under UHV.

We find spectra that are reminiscent of solid state spectra for multilayers of QA on Ag(100). In addition, we see blue-shifted spectra for highly dilute QA layers (0.0005 ML – 0.1 ML) with a multitude of spectral features. We find that the stability of these spectral features under laser illumination varies depending on the thickness of the underlying KCl layer. Spectra are stable at 13 K for QA on 3-4 layers of KCl. However, on 6-8 layers of KCl, a spectral red-shift and a loss of FL-intensity is induced upon laser illumination at 13 K. We attribute these findings to a diffusion barrier of QA on KCl films that is dependent on the KCl-film thicknesses because the long-range interactions with the Ag(100) substrate are relevant [2].

[1] Phys. Rev. Lett. 2023, **130** (12), 126202.

[2] J. Phys. Chem. C 2023, **127** (49), 23814-23826.

This work was supported by the DFG through the research training group 2591.

O 46.10 Tue 18:00 P2

**Field driven crossover of bonding and antibonding states in excitonic aggregates** — •Amandeep Sagwal[1,2], Rodrigo Cezar De Campos Ferreira[1,3], Petr Kahan[1], Tomáš Neuman[1], and Martin Švec[1,3] — [1]Institute of Physics, Czech Academy of Sciences — [2]Faculty of Mathematics and Physics, Charles University; Czech Republic — [3]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

The present study aims to examine the effect of an electric field on the excitonic states of chromophore aggregates confined in optical nanocavity of a low-temperature SPM. Utilizing an optical configuration intended for near-field spectroscopies, tip-enhanced photoluminescence (TEPL) is used to investigate PTCDA molecules, deposited on a thin decoupling layer of NaCl on Ag(111) surface. A different energy shift is observed consistently between the bonding and antibonding excitonic emission lines in the spectra of dimer, trimer, and tetramer aggregates, in some cases even leading to a crossover. Typically, the antibonding states manifest a larger blue shift with increasing positive bias voltage applied on the gate electrode (substrate). We discuss the phenomenon using TD-DFT simulations and many-body state diagrams.

O 46.11 Tue 18:00 P2

**Near-field spectroscopy of vibronic states of molecular aggregates** — •Sidhartha Nayak[1], Fulu Zheng[2], and Alexander Eisfeld[1] — [1]MPIPKS, Dresden, Germany — [2]Department of Physics, Ningbo University, Ningbo, China

Strong dipole-dipole interactions between molecules give rise to delocalized electronic excited states in molecular aggregates, which determine their optical properties such as absorption. In near-field spectroscopy, the absorption spectrum of an aggregate is obtained when the molecules interact with electromagnetic radiation that is inhomogeneous across the length of the aggregate. Theoretically, by considering the near-field radiation from the apex of a metallic tip as a source of a localized field, it has been shown that the spectra of the aggregate reveal it's purely electronic states that are inaccessible through traditional far-field methods [1, 2]. In this contribution, we study aggregates composed of molecules with internal vibrational modes that are strongly coupled to electronic excitations, leading to non-Markovian phenomena. Using a local field method, which is numerically inexpensive, we observe that the vibronic states of aggregates are revealed in the near-field spectra and the spectra are comparable to those obtained by using a more accurate but computationally intensive method [3].

[1] X. Gao and A. Eisfeld, *J. Phys. Chem. Lett.* 9, 6003 (2018)

[2] S. Nayak, F. Zheng and A. Eisfeld, *J. Chem. Phys.* 155, 134701 (2021)

[3] D. Suess, A. Eisfeld and W. T. Strunz, *Phys. Rev. Lett.* 113, 150403 (2014)

O 46.12 Tue 18:00 P2

**The Luminescence of Rylene Derivatives** — •Petr Kahan[1], Rodrigo Ferreira[1,2], Amandeep Sagwal[1], Jiří Doležal[2], and Martin Švec[1,2] — [1]Institute of Physics, Czech Academy of Sciences — [2]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

The exploration of single-molecule luminescence using scanning tunneling microscopy (STM) is a vividly developing area of research. A number of works using STM-PL/EL and TERS techniques addressing the photophysics at the true single-molecule limit have employed rylene dyes for their known luminescent properties [1,2]. However, up to this point, a thorough comparison investigating the absorption and luminescent characteristics of molecules that share similar rylene-based configurations has not been carried out. This study presents a comparative analysis with the tip-enhanced spectromicroscopy in STM nanocavity on isolated molecules such as NTCDA, PTCDA, and DBP [3]. The findings reveal surprisingly distinct characteristics of each species; notably of their photoluminescence (PL) fingerprints and photocurrent maps. This shows the versatility of chemically related species, which holds promise for tailoring custom optoelectronic functionality in molecular aggregates.

[1] Doležal, J. et al. ACS Nano 16, 1082*1088 (2022). [2] Kimura, K. et al. Nature 570, 210*213 (2019). [3] Kröger, J. et al. Nano Lett. 18, 3407*3413 (2018).

O 46.13 Tue 18:00 P2

**Spin Hall Magnetoresistance as a Probe for Chiral-Induced Spin Selectivity** — •Simon Sochiera[1], Ashish Moharana[1], Yael Kapon[2], David Anthofer[1], Fabian Kammerbauer[1], Akashdeep Akashdeep[1], Shira Yochelis[2], Mathias Kläui[1], Yossi Paltiel[2], and Angela Wittmann[1] — [1]Institute for Physics JGU, Mainz, Germany — [2]Hebrew University of Jerusalem, Jerusalem, Israel

Chiral molecules have gained significant attention in the spintronics community due to their ability to polarize electron spin angular momentum without any heavy metal atoms via the chiral-induced spin selectivity (CISS) [1] effect. Several optical and electrical methods confirmed the CISS effect. However, despite numerous theoretical approaches, the fundamental mechanisms of the CISS effect are still an open question. A recent experiment [2] reported a significant modulation of spin-to-charge conversion with chiral molecules in a spin-pumping experiment. Building on this result, we create a hybrid structure by combining a well-established spin Hall magnetoresistance (SMR) experiment with chiral molecules. The SMR relies on the reflection and absorption of spin currents at interfaces adjacent to a layer exhibiting an (inverse) spin Hall effect, such as a heavy metal. This allows for direct probing of the spin-to-charge conversion modulation by chiral molecules. Combined with the results established in the spin-pumping experiment, this paves the path toward designing new chiral-molecule-based spin-torque devices.

[1]: R. Naaman et al., Nat. Rev. Chem. 3, 250 (2019)

[2]: A. Moharana et al., arXiv:2402.19246 (2024)

## O 47: Poster Electron-driven Processes

Time: Tuesday 18:00–20:00 Location: P2

O 47.1 Tue 18:00 P2

**Non-equilibrium electron distribution effects in ultrafast light-driven desorption dynamics** — •Matthew Larkin, Henry Snowden, and Reinhard J. Maurer — University of Warwick, Coventry, UK

At metal surfaces, light excitation drives electronic states out of the (thermal) Fermi-Dirac distribution. The resulting non-equilibrium electronic distribution can induce coupled electron-nuclear dynamics that lead to ultrafast structural processes such as light-driven desorption of molecules. As non-equilibrium electron distributions in metals are short-lived, their role in the mechanics of light-driven surface dynamics remains insufficiently understood. In this work, we perform mixed quantum-classical dynamics simulations using a variant of the trajectory surface hopping method where electrons and nuclei are propagated simultaneously and electronic transitions between hundreds of electronic states can be captured. We describe light-generated nonthermal electron distributions as initial conditions to those dynamics. For simple 1D and 2D model systems of atomic and molecular desorption from metal surfaces, we study the role of non-thermal electrons by simulating light-driven desorption probabilities for comparable thermal and non-thermal electronic distributions and discuss the future applicability of this approach for high-dimensional dynamics.

O 47.2 Tue 18:00 P2

**Spin effects in ultrafast non-equilibrium dynamics at surfaces** — •Ash Baldwin and Reinhard J. Maurer — University of Warwick, Coventry, United Kingdom

Energy, charge, and spin transfer are important factors in modelling ultrafast gas-surface dynamics such as hyperthermal scattering and light-driven dynamics at surfaces. In particular, on metal surfaces, nonadiabatic energy dissipation is an important energy transfer channel in atomic and molecular dynamics at surfaces. In cases of adsorbates with unpaired spin, an additional question arises if and under which conditions the spin moment of the adsorbate survives the scattering event. The challenge lies in capturing the explicit electron correlation in the electronic structure and its effect on the coupled electron-nuclear motion, which mean-field dynamics methods cannot fully capture.

Here, we model the fate of adsorbate spin during scattering from a metal surface using the Newns-Anderson model. We go beyond previous works by simulating the nuclear dynamics beyond mean-field Ehrenfest dynamics, using stochastic trajectory surface hopping methods. Our model is applied to study the spin survival probability of hydrogen atoms on copper and platinum as a function of various model parameters and initial conditions such as the adsorbate kinetic energy and the adsorbate-metal coupling strength to identify the regime in which a finite spin survival probability can be measured.

O 47.3 Tue 18:00 P2

**Adsorbate motors: toward tuning unidirectionality by chemical functionalisation** — •Grant J Simpson[1], Mats Persson[2], and Leonhard Grill[1] — [1]University of Graz, Austria — [2]University of Liverpool, UK

The purpose of a molecular motor is to convert external energy into unidirectional motion. Feringa-type molecular motors, in which double-bond isomerisation leads to large geometric changes in the molecule, are known to undergo rapid unidirectional motion in solution but often have a reduced function when adsorbed on a surface. In contrast, recently discovered adsorbate motors [1] do not exhibit large structural changes and thus their motion is efficient and unidirectional when adsorbed on a metal surface. Using a scanning tunnelling microscope (STM), we track such motion at the single-molecule scale. The motion is triggered by an internal proton transfer reaction. We further show that, by altering the local chemical structure, this tautomerisation can be affected and may result in modulation of the unidirectional molecular translation.

[1] G. J. Simpson, M. Persson, L. Grill, Nature, 621, 82-86 (2023)

O 47.4 Tue 18:00 P2

**Creation, Displacement, and Dynamics of Individual Phasons on Si(001)** — •Gaël Reecht, Michael Horn-von Hoegen, and Manuel Gruber — Universität Duisburg-Essen, Duisburg, Germany

The Si(001) surface, characterized by buckled dimers resulting from dangling bond pairing, exhibits a variety of structural configurations. The energetically favorable c(4x2) reconstruction can be manipulated into the p(2x2) configuration, differing by a glide of adjacent rows. The interface between these two phases is known as a phason [1]. Despite its significance in structural phase transitions, the mechanisms driving phason propagation remain poorly understood.

In this study, we employ low-temperature scanning tunneling microscopy to explore the diffusion of individual phasons under tip-induced excitation. We systematically examine the effects of tunneling current, bias voltage, and electric field on the formation and displacement of these structural defects. Phason motion below the STM tip results in stochastic jumps in tunneling current, which we analyze through time-resolved measurements. These findings shed light on the displacement dynamics of phasons and enhance our understanding of the underlying processes. We gratefully acknowledge funding from the CRC1242. [1] Y. Pennec et al., Phys. Rev. Lett., 96, 026102 (2006).

O 47.5 Tue 18:00 P2

**Triplet exciton dynamics at the tetracene/a-Si/c-Si(111) interface** — •Marvin Krenz[1,2], Simone Sanna[1], Wolf Gero Schmidt[2], and Uwe Gerstmann[2] — [1]Institut für Theoretische Physik, Justus-Liebig Universität Gießen, 35392 Gießen, Germany — [2]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

Exciton transfer is highly relevant for many physical, chemical, and biological processes. The transfer of triplet excitons across the tetracene-silicon interface in sensitized solar cells is a recent example in this context [1]: The excitons, generated by singlet fission in tetracene (Tc), promise to increase the cell efficiency from the single-junction limit of 29% to values as high as 35% [2]. In a previous work, we showed the significance of dangling bond (db) defects for the triplet transfer [3] at a model interface, where tetracene was bonded to an ideal c-Si(111) surface. Here, we present ab initio calculations for a more realistic structure, with a thin film of amorphous silicon (a-Si:H) in-between, resulting in a Tc/a-Si/c-Si model structure. We find that dbs are vital for the exciton transfer also in this case. Dbs at the a-Si/c-Si interface or in the a-Si interlayer itself affect the exciton transfer differently. Generally, it is found that the a-Si layer is energetically favourable for excitation transfer. However, the exciton electron tends to be trapped in a-Si conduction band tail states. Thus, the exciton transfer requires an external field to be completed. [1] M. Einzinger et al. Nature 571, 90*94 (2019). [2] A. Rao et al., Nat. Rev. Mater. 2, 17063 (2017). [3] M. Krenz et al., Phys. Rev. Lett. 132, 076201 (2024)

# O 48: Poster Surface Dynamics

Time: Tuesday 18:00–20:00 Location: P2

O 48.1 Tue 18:00 P2

**Atomistic modeling of ultrafast laser induced structural changes in Bismuth** — •Sahar Bakhshi Sangari, Jimiben Patel, Bernd Bauerhenne, and Martin Garcia — Institute of Physics, University of Kassel, Kassel, Germany

We present a temperature-dependent interatomic potential for laser-excited bismuth, $\Phi_{Bi}(Te)$, developed using a database of temperature-dependent density functional theory (DFT) calculations. Bismuth is a widely studied material in experiments, yet theoretical studies exploring its atomic dynamics following femtosecond laser excitation remain scarce. Our work compares the physical properties predicted by $\Phi_{Bi}(Te)$ with those obtained from ab initio simulations, demonstrating its reliability. We use $\Phi_{Bi}(Te)$ to describe, in the framework of a generalized two-temperature-model molecular dynamics (TTM-MD) method, laser induced thermal and nonthermal ultrafast structural changes in Bi. We compute the time evolution of selected Bragg peaks and directly compare them with experimental observations. This approach enables efficient and accurate modeling of complex material behaviors, providing a valuable alternative to computationally intensive temperature-dependent DFT simulations.

O 48.2 Tue 18:00 P2

**Design and Characterization of Optical Cavities for Light-Induced Phase Transitions in Indium-Based Peierls Insulators** — •Florian Spickmann[1,2], Sierra Randall Heinrich[1,2], Sebastian Zafra Koch[1,2], Murat Sivis[1,2], Hannes Boeckmann-Clemens[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

The integration of quantum materials into optical cavities enables active control of their properties through enhanced light-matter interactions. Low-dimensional materials, such as Peierls insulators, are particularly sensitive to external stimuli, making them ideal candidates for such studies [1]. This work focuses on designing and fabricating optical resonators on (111) silicon membranes, including slab waveguides, ridge waveguides, and ring resonators. The structures are created using focused ion beam (FIB) milling and electron beam lithography (e-beam), with light coupling achieved via integrated gratings. Characterization of the resonators is performed using Fabry-Pérot interferometry. Future studies will employ ultrafast low-energy electron diffraction (ULEED) to visualize light-driven phase changes in indium wires localized on these optical resonators, representing a promising model system for cavity-controlled light-matter interaction in condensed matter.

[1] Böckmann, Hannes, et al., Structural Dynamics 9.4 (2022)

O 48.3 Tue 18:00 P2

**Ultrafast LEED Study of Bismuth Thin Films on Silicon (001)** — •Nandana V Uday[1], Felix Kurtz[1], Jonas Fortmann[3], Alp Akbiyik[1], Michael Horn-von-Hoegen[3,4], and Claus Ropers[1,2] — [1])Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany — [2]4th Physical Institute ,Solids and Nanostructures, University of Göttingen, 37077 Göttingen, Germany — [3]University of Duisburg-Essen, 47057 Duisburg, Germany — [4]Center for Nanointegration (CENIDE), 47057 Duisburg, Germany

The interface between two materials in a heterostructure serves as a barrier to the diffusion of thermal energy, thereby hindering heat flow across the boundary. On the nanoscale, heat transport may further be modified. Recently, it was shown that the thermal transport from Bi film into a Si substrate is reduced for films thinner than the phonon mean free path, due to phonon trapping by total internal reflection [1]. To study the non-equilibrium phonon dynamics in this process, ultrafast low-energy electron diffraction (ULEED) is suitable and direct means providing ultrafast temporal and high momentum resolutions. By analyzing the momentum-resolved map of a transient inelastic scattering background [2], we aim to identify phonon trapping, depopulation, and thermalization. As a first step, we monitor the heat transfer by phonons through the thin film-substrate interface, extracting cooling times from the transient lattice temperature of the bismuth film.

O 48.4 Tue 18:00 P2

**Predicting and modelling incommensurate charge density waves in 1H-TaSe$_2$ via downfolding approach** — •Clara Pfister[1,2], Laura Pätzold[1], and Tim O. Wehling[1,2] — [1]I. Institute of Theoretical Physics, U Hamburg — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg

Studying the emergence and thermodynamic behaviour of symmetry-broken phases such as charge density waves (CDWs) in solids is of great interest to deepen our understanding of collective phenomena and interactions between electrons and the crystal lattice. Incommensurate CDWs (ICCDWs) are especially intriguing because a realistic and efficient computational method to predict them has not been developed yet. To model ICCDW phases in the exemplary transition metal dichalcogenide material 1H-TaSe$_2$, we employed a downfolding approach that reduces the electronic degrees of freedom by retaining only the low-energy subspace relevant to CDW formation. This method achieves a computational speed-up of approximately five orders of magnitude compared to purely ab initio calculations [1], making it possible to simulate sufficiently large supercells efficiently. Our approach allows for modelling the ICCDW with reasonable accuracy, with the predicted temperature range for its occurrence agreeing well with experimental results of the ICCDW in undoped 2H-TaSe2 [2]. This suggests that our approach is applicable for the description of other materials exhibiting ICCDWs.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)

[2] X. Shen et al., *Nat. Commun.* **14**, 7282 (2023)

# O 49: Poster Nanostructures at Surfaces

Time: Tuesday 18:00–20:00 Location: P2

O 49.1 Tue 18:00 P2

**Au induced nanostructures on Si(110)** — •Stephan Appelfeller — MAX IV Laboratory, Lund University, Sweden

The deposition and annealing of small amounts of Au on clean Si substrates often lead to enticing nanostructures showing, e. g., spin ordering on vicinal Si(111) substrates or self-doping by adatoms on planar Si(111). A curious case are Au induced nanostructures on Si(110) for which the phase diagram is known in the submonolayer to monolayer regime, but for which few detailed studies exist, although, quasi-1D metallicity has been proposed for one of the nanostructures.

Here, the various nanostructures and their evolution are studied in real space using scanning tunnelling microscopy measured in MAX IVs SPM Support Lab, with core-level and angle-resolved photoemission spectroscopy obtained at the FlexPES beamline of the MAX IV Laboratory. For lowest Au coverages, a 2x1 superstrusture showing a distinct Au 4f core-level component forms. With increasing Au coverage, rows of 2x3 subunits develop leading to the formation of the 2x5 reconstruction with quasi 1D-metallicity and the two-domain (4,0)x(±1,3) high coverage phase, which shows a high stability and recoverability in UHV. This stability is shared with Au silicide nanowires, which grow in the mono- to multilayer Au coverage regime. Since there are no stable bulk Au silicides, the observation of Au silicide nanowires is a beautiful reminder that surfaces and interfaces in general are different and often deviate from bulk expectations.

O 49.2 Tue 18:00 P2

**XPS study of CuO, WO3 and CuWO nanoparticles-based films** — •Michal Procházka[1], Kalyani Shaji[2], Stanislav Haviar[2], Eliška Benediktová[2], Radomír Čerstvý[2], Ján Minár[1], Petr Zeman[2], and Jiří Čapek[2] — [1]New Technologies - Research Centre, University of West Bohemia, Univerzitní 8, Plzeň, 301 00, Czech Republic — [2]Department of Physics and NTIS - European Centre of Excellence, University of West Bohemia, Univerzitní 8, Plzeň, 301 00, Czech Republic

Interest in clean and sustainable technologies is rapidly growing and hydrogen is widely used in this field. With this development, more emphasis is placed on hydrogen gas sensors as hydrogen poses significant risks due to its explosive nature and flammability [1]. Structural parameters and surface properties plays a significant role in interaction of gas with sensor material [2]. Therefore, the nanoparticles of various materials are more and more explored. To understand the surface evolution after annealing in the air we measured XRD, SEM and XPS of CuO, WO3 and CuWO nanoparticles-based films prepared by magnetron-based gas aggregation technique.

[1] P. S. Chauhan, S. Bhattacharya, Hydrogen gas sensing methods, materials, and approach to achieve parts per billion level detection: A review, Int. J. Hydrogen Energy. 44 (2019) 26076-26099.

[2] H. Zhao, Y. Wang, Y. Zhou, Accelerating the Gas-Solid Interactions for Conductometric Gas Sensors: Impacting Factors and Improvement Strategies, Materials. 16 (2023).

O 49.3 Tue 18:00 P2

**Hydroxyl Groups on Different Metal Doped $Co_3O_4$ Particle Catalysts Observed by Sum Frequency Generation Vibrational Spectroscopy** — •Furong Yan[1], Carsten Placke-Yan[2], Zhipeng Huang[1], Yujin Tong[1], and R. Kramer Campen[1] — [1]Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen — [2]Faculty of Chemistry and Institute of Inorganic Chemistry, University of Duisburg-Essen

Metal-doped $Co_3O_4$ nanoparticles are promising catalysts for the electrochemical oxygen evolution reaction (OER), with surface Co-OH groups playing a critical role in the water oxidation cycle. However, the influence of metal doping on the behavior of surface OH groups and its subsequent effect on OER activity remains uncertain.

Here, we investigate the effects of metal doping (Mn and V) on the bonding of OH groups using sum frequency generation (SFG) vibrational spectroscopy. Our results reveal that Mn-doped $Co_3O_4$ exhibits stronger bonding between OH groups and the surface compared to both pristine $Co_3O_4$ and V-doped $Co_3O_4$, leading to a reduction in OER activity. We propose two mechanisms: (1) an excess of OH groups can block active sites and increase charge transfer resistance, and (2) the stronger Co-OH bonds in Mn-doped $Co_3O_4$ may hinder the cleavage of Co-OH bonds, thereby impeding the OER process. These findings provide valuable insights into how surface interactions with OH groups can be tailored to optimize OER catalytic performance.

O 49.4 Tue 18:00 P2

**Coral-like structures on nickel surfaces obtained by nitrogen plasma treatment** — •Christina Meinert, Timo Wagner, Felix Schaumburg, Moritz Sünner, Nicolas Wöhrl, and Axel Lorke — Faculty of Physics, University Duisburg-Essen

For electrochemical processes, nickel sheets are commonly used as electrode material because of their low cost and easy handling. Here we report on the use of a microwave induced remote nitrogen plasma to change the surface of the nickel, improving the electrochemical and mechanical properties of the nickel electrode. During this process the surface obtains coral-like nanostructures and a nitridation of the nickel can be detected. AFM is employed to characterize these evolved nanostructures. Furthermore, EDX, Raman Spectroscopy and XPS are used to identify the chemical composition of the surface. In addition, wettability is probed as this is important for the efficiency of electrolysis. The plasma process is also applied to more complex surfaces than nickel plates such as wires and meshes. This allows to investigate the feasibility and limitations of treating these substrates.

O 49.5 Tue 18:00 P2

**Exploring Topological Boundary Modes in Atomically Assembled Quantum Structures** — •Adrian Weindl, Christoph Setescak, and Franz J. Giessibl — Faculty of Physics, University of Regensburg, D-93053 Regensburg, Germany

Single-atom and single-molecule manipulation enables the construction of quantum simulators: artificial structures assembled atom-by-atom or molecule-by-molecule to emulate key properties of complex systems that are challenging or impossible to fabricate directly. Using scanning tunneling microscopy (STM) and atomic force microscopy (AFM), we create two atomic-scale structures from individual CO molecules on Cu(111): a 1D Su-Schrieffer-Heeger (SSH) chain and a 2D Kagome lattice.

The 1D SSH chain represents a fundamental system capable of hosting topological boundary modes. We investigate the interaction between these boundary modes and the AFM tip. As the boundary modes are spatially localized and pinned in energy, they are not expected to undergo chemical bonding, unlike the bulk states of the chain, which may exhibit such interactions.

The 2D Kagome lattice on Cu(111) was initially proposed as a higher-order topological insulator, a classification that remains under debate. Through STM and AFM measurements, we aim to contribute to this ongoing discussion by introducing defects and analyzing the bonding behavior of the purported topological corner modes.

O 49.6 Tue 18:00 P2

**Au vs. Ag: How Does the Choice of Substrate Influence the Formation of SAMs with Carboxylic Head Groups?** — •Verena Müller[1], Julian Picker[1], Daniel Hüger[1], Christof Neumann[1], Marco Gruenewald[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]Friedrich Schiller University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

Self-assembled monolayers (SAMs) enable modification of various solid substrates at the molecular level, providing a wide range of applications in nanoscience and nanotechnology, *e.g.*, photonics, organic electronics and biochemical sensing.

In this contribution, we present a systematic investigation of the formation of SAMs with carboxylic head groups (–COOH) on Ag and Au substrates. To this end, we analyze the results for three molecular precursors: a $Ru^{II}$-polypyridine complex photosensitizer, hexadecanoic acid and *p*-terphenyl-4-carboxylic acid. Complementary surface science characterization methods - including X-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED), scanning tunneling microscopy (STM) and polarization-modulation infrared reflection absorption spectroscopy (PM-IRRAS) - were employed to confirm the successful SAM formations. The obtained results are utilized to gain insight into the nature of the chemical interaction between the carboxylate and the metal surface.

O 49.7 Tue 18:00 P2

**Phase Transitions of Naphthalene-2,3-carbonitride Steered by Solvent Effects and Metal Ion Concentration Variation** — •Longnan Yu[1], Li Wang[2], and Xiaoqing Liu[3] — [1]KIT, Karlsruhe, Germany — [2]Nanchang University, Nanchang, China — [3]Nanchang University, Nanchang, China

This study explores the structural phase transitions of naphthalene-2,3-carbonitride (2,3-DCN) on highly oriented pyrolytic graphite (HOPG) influenced by varying solvents and Cu2+ ion concentrations. By combining scanning tunneling microscopy and density functional theory, it is revealed that in 1-nonanoic acid,Cu2+ ions coordinate with 2,3-DCN and other ligands (Cl- or 1-nonanoic acid), forming structures with a coordination number of 4 that depend on the 2,3-DCN to Cu2+ molar ratio. In contrast, in 1-heptanoic acid,Cu2+ ions do not coordinate with 2,3-DCN, and phase transitions occur solely through altered hydrogen bonding. This work highlights solvent-dependent metal organic coordination as a novel strategy for tailoring nanoarchitectures.

O 49.8 Tue 18:00 P2

**Bottom-up realization of quasi-1D electronic states from Cs atoms on InSb(110)** — •Niek Aarts, Annique Krieg, Emil Sierda, Danis Badrtdinov, Brian Kiraly, Elze Knol, Gerrit Groenenboom, Mikhail Katsnelson, Malte Rösner, Daniel Wegner, and Alexander Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

1D-electronic systems are predicted to exhibit very different physical phenomena compared to 2D and 3D systems. Scanning tunnelling microscopy (STM) and spectroscopy (STS) provide a way to study 1D electronic systems on surfaces in a bottom-up approach with atomic-scale precision by utilising atomic manipulation.

Here, we study the electronic states of quasi-1D structures that result from coupling individual Cs atoms adsorbed on InSb(110) using low-temperature STM and STS. When constructing chains of Cs atoms, we observe the formation of quantized electronic states in energy with a modulated charge density along the chain. We can tune these electronic states by changing the length and Cs density of the chain. Modifying the chain length, changes the spacing of the electronic states. Changing the density of Cs atoms, changes the onset energy of the electronic states. We ascribe these observations to a 1D-particle in a box behavior for the lowest electronic states. For the electronic states at higher energy, we observe deviations from the simple particle in a box description. These deviations could be due to the onset of states with a higher order orbital symmetry or due to a coupling of these states to a bath.

O 49.9 Tue 18:00 P2

**Investigation of onset field variations in annealed and as-deposited NbTiN samples through field emission scanning microscopy** — •Frederic Braun[1], Isabel Díaz-Palacio[2], Lea Preece[2], Florian Brockner[1], Robert Zierold[2], Marc Wenskat[2], Wolfgang Hillert[2], and Dirk Lützenkirchen-Hecht[1] — [1]Bergische Universtiät Wuppertal — [2]Universität Hamburg

Current superconducting radio frequency (SRF) cavities are predominantly constructed from high purity Niobium which is pushed to its theoretical limit. To enhance future cavity performance by minimizing operational power losses and increasing accelerating field strength, the focus of research must shift to alternative cavity materials. An effective strategy involves depositing superconducting thin films like NbTiN or Nb3Sn on the cavity inner walls. Heat treating NbTiN may further optimize film properties. In this study various samples, including as deposited NbTiN and annealed NbTiN are analyzed via a Field Emission Scanning Microscopy (FESM). Current-voltage-curves allow the determination of onset-fields for parasitic field emission . Mapping these fields at e.g., 1 nA reveals lateral variations due to thin film inhomogeneities, defects or surface contaminations Additionally, assessing long term surface stability through constant current measurements over an extended period is crucial for practical cavity applications.

O 49.10 Tue 18:00 P2

**Surface Reconstructions and Photocatalysis of Thermally Reduced $LiNbO_3$ and $BaTiO_3$ Single Crystals** — •Marta Macyk[1], Andrzej Jasicki[1], Llorenç Albons[2], Konrad Szajna[1], Martin Setvin[2], Dominik Wrana[1], and Franciszek Krok[1] — [1]Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland — [2]Department of Surface and Plasma Science, Charles University, Prague, Czech Republic

Perovskite oxides, such as $BaTiO_3$ (BTO) and $LiNbO_3$ (LNO), exhibit a wide range of different stoichiometries and crystal structures that make them ideal candidates for applications in optoelectronics and catalysis. Their properties can be tuned by the change of stoichiometry and the introduction of oxygen vacancies achieved by annealing under Ultra High Vacuum (UHV).

This poster presents a comparative study of surface reconstructions for tetragonal $BaTiO_3(001)$ and hexagonal $LiNbO_3(0001)$ after UHV annealing under low oxygen partial pressure. LEED analysis reveals a $(1\times1)$ to $(\sqrt{5}\times\sqrt{5})R26.6°$ transition for BTO, while LNO undergoes a $(1\times1)$ to $(\sqrt{3}\times6)R30°$ transition, ending with $(3\times3)$ structure at temperatures near 1200°C. Morphological studies using SEM, STM, and AFM show the formation of nanowire structures aligned with the substrates' crystallographic directions, offering insights into controlled surface engineering. Furthermore, photocurrent measurements at variable temperature were performed on the thermally modified crystals to evaluate their photocatalytic and pyrocatalytic activity under ambient conditions.

O 49.11 Tue 18:00 P2

**Freestanding thin film cryo-EM samples for electrospray ion beam deposition and molecular imaging** — •Stephanie Stankard, Stephan Rauschenbach, Lukas Eriksson, and Jingjin Fan — Department of Chemistry, University of Oxford

Over the past decade, cryogenic electron microscopy (cryo-EM) has become the dominating method for imaging in structural biology, a method in which samples are conventionally made by plunge freezing.

Combining cryo-EM with soft landing, electrospray ion beam deposition (ES-IBD) is a novel approach where intact, folded protein gas phase ions are landed onto the cryo-EM samples. For this, supported grids are required, which also need to be electron-transparent, and conductive. Often also ice needs to be grown on them after protein deposition.

Here, we present an analysis and optimisation of various thin, freestanding, amorphous carbon films for the purpose of application as a ESIBD and cryo-EM substrates.

## O 50: Poster Organic Molecules on Inorganic Substrates: Adsorption and Growth

Time: Tuesday 18:00–20:00 Location: P2

O 50.1 Tue 18:00 P2

**Polymorphism of Naphthalene on Ag(111) in and out of thermodynamic equilibrium** — •Lorenz Brill[1], Christoph Wachter[2], Roman Forker[1], Oliver T. Hofmann[2], and Torsten Fritz[1] — [1]Friedrich-Schiller-Universität, Jena, Germany — [2]Technische Universität, Graz, Austria

Even with a seemingly simple molecule like naphthalene, a rich polymorphism has been observed on Cu(111). Additionally, calculated phase diagrams predict multiple different structures of naphthalene on Ag(111), depending on the pressure and temperature during naphthalene deposition. In this poster, we present first experimental results of naphthalene structures formed in thermodynamic equilibrium obtained in our custom chamber specially designed to enable molecular growth in thermodynamic equilibrium. We compare our results to naphthalene structures grown using a conventional setup.

O 50.2 Tue 18:00 P2

**Coverage-dependent assembly of functionalized helicenes** — •Elise Fürch[1], Jonas Brandhoff[1], Fumi Nishino[2,3], Keisuke Fukutani[2,3], Marco Gruenewald[1], Maximilian Schaal[1], Felix Otto[1], Roman Forker[1], Takashi Hirose[4], Satoshi Kera[2,3], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute for Molecular Science, Myodaiji, 444-8585, Okazaki, Japan — [3]The Graduate University of Advanced Studies, Hayama-cho, 240-193 Kanagawa, Japan — [4]Institute of Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan

Recently, the interest in chiral molecules has spiked. The chirality-induced spin selectivity (CISS) promises a high spin-polarizability for electrons traversing a chiral molecule. However, the CISS effect is yet not fully understood. To be able to probe the CISS effect with area averaging methods like photoelectron spectroscopy a well-defined chiral thin film, consisting of helical molecules, is needed. In this study the chiral molecule thiadiazole[9]helicene (TD[9]H) is investigated on Au(111) and Ag(111) surfaces. To understand how chirality from one single molecule evolves into a fully chiral overlayer, a coverage dependent study, showing different structural motifs of TD[9]H, was performed. This structural evolution was investigated using scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). In combination, these methods reveal a chiral lattice, and the role of the different molecule-molecule and molecule-substrate interactions will be discussed.

O 50.3 Tue 18:00 P2

**Determining the Epitaxial Relations of Lead Phthalocyanine on Graphitic Surfaces** — •Marco Gruenewald, Roman Forker, Matthias Spoddeck, and Torsten Fritz — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

The epitaxial relations between lead phthalocyanine (PbPc) layers and single-crystal graphite (SCG) as well as few-layer graphene/SiC(0001) are determined. Compared to previous reports, we obtain a clearly improved precision by combining the following concepts: [i] the use of distortion-corrected, calibrated low-energy electron diffraction (LEED), [ii] the complementary use of large-scale scanning tunneling microscopy (STM) with high resolution, [iii] the evaluation of multiple scattering features in LEED and Moiré spots in Fourier-transformed STM images, [iv] the simulation of those reciprocal-space patterns with an objective numerical fitting to the experimentally discernible spots, and [v] the analysis of the STM Moiré patterns in real space. Our independently determined LEED and STM results mutually confirm each other due to the remarkably similar structural parameters obtained. For all systems investigated we find noncommensurate, point-on-line coincident registries, and the epitaxial relations of PbPc layers on SCG and on graphene/SiC(0001) are found to be nearly identical despite the different compositions of those substrates. https://doi.org/10.1021/acs.cgd.4c01055

O 50.4 Tue 18:00 P2

**Solvent-Free Fabrication of Supported Lipid Bilayers Incorporating Carbon Quantum Dots and Gramicidin A for Biosensing Applications** — •Daniel A. Saavedra[1], Benjamín Ruz[1], Nicolás Moraga[1], Nancy Gomez-Vierling[1], Marcelo A. Cisternas[2], Susana D. Rojas[2], and Ulrich G. Volkmann[1] — [1]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]Escuela de Ingeniería Industrial, Univ. de Valparaíso, Chile

This study employed two phospholipids for the formation of supported lipid bilayers (SLBs): DPPG, with a net negative charge for enhanced adsorption to surfaces and biomolecules, and DPPC, which is neutral. SLBs were fabricated using a solvent-free, dry, ultra-high vacuum (UHV) approach [1], designed for protein insertion and nanoscale biosensor development for Forster energy transfer (FRET) detection mechanism.

Gramicidin A, a stable ion-channel protein, was incorporated into SLBs via physical vapor deposition monitored by high-resolution ellipsometry, followed by thermal treatment to enhance stability. Carbon quantum dots (CQDs), synthesized through hydrothermal carbonization of chitosan, were added via spin-coating. CQDs were selected for their photostability, low toxicity, and tunable fluorescence [2].

Acknowledgements: ANID Ph.D. Fellowships (DAS, NM, NGV), PUENTE-UC 2024-25. References: [1] Cisternas, M.A. et al., IJMS, 21, 6819 (2020). DOI: 10.3390/ijms21186819 [2] Wu, Q., et al., Nano Research, 16, 1835-1845 (2023). DOI: 10.1007/s12274-022-5189-2

O 50.5 Tue 18:00 P2

**Long range ordering of molecular layers on Ag(110)** — •Ravi Priya, Weishan Wu, and Peter Jakob — Department of Physics, Philipps University of Marburg, Germany

Single domain molecular layers have been explored on the non-hexagonal Ag(110) substrate in terms of their long-range ordering using SPA-LEED and vibrational signature using high-resolution FT-IRAS. The absence of rotational domains for fcc(110) metal substrates allows for growing layers with uniform azimuthal orientation of deposited molecules. We have investigated various molecules and configurations that may form single domain molecular layers (including mirror domains). Specifically, monolayers of PTCDA, NTCDA, and regio-selectively substituted pentacene species (pentacene (PEN), pentacene-quinone (P2O), pentacene-tetrone (P4O), quinacridone (QA)) were deposited on Ag(110) and examined in terms of their structure using SPA-LEED, and their vibrational signature using IR - spectroscopy. Among them, PTCDA, NTCDA, PEN, and QA have been found to form parallel-oriented, single domain structures. For QA two novel heterochiral phases are found after annealing, in addition to the single-domain homochiral phase present $T < 500$K. For P2O and P4O, steric hindrance and hydrogen bonding lead to the formation of 1D islands and 2D islands, respectively, at sub-monolayer coverages. Another finding refers to the increased molecule - metal interaction on Ag(110) vs. Ag(111) that leads to an extra energy (down)shift of the LUMO, thereby having a significant impact on interfacial dynamic charge transfer (IDCT) of vibrational modes.

O 50.6 Tue 18:00 P2

**Structural and vibrational properties of mixed (CuPc + P4O) molecular layers on Ag(111)** — •Yeondu Kim, Ravi Priya, and Peter Jakob — Department of Physics, Philipps University Marburg, Germany

Structural properties of mixed layers comprising CuPc and P4O on Ag(111) and their thermal evolution have been investigated by means of Fourier-transform infrared absorption (FT-IRAS) and electron diffraction (SPA-LEED). For this material combination several long-range ordered phases at different relative ratios are found. Their formation and thermal stability have been analyzed in the temperature range 80 - 500 K, limited by thermal desorption and/or dissociation of the CuPc and P4O compounds at high temperature. Lateral interactions between CuPc and P4O within the mixed layers lead to characteristic frequency shifts of out-of-plane modes. In parallel, the intensities of in-plane vibrational modes of CuPc and P4O are strongly attenuated when adsorbed at nearby locations, indicating a major change in the associated interfacial dynamical charge transfer (IDCT). Specifically, IDCT that is quite prominent for the pure CuPc/Ag(111) and P4O/Ag(111) monolayers, is substantially attenuated for the mixed layers. This is ascribed to a through-metal charge transfer from CuPc to P4O that is associated with an upshift of the CuPc former LUMO and the correlated downshift of the P4O former LUMO. These correlated shifts lead to substantially lower density of states at the fermi level for both molecular species and thereby a weakening of IDCT induced bands.

O 50.7 Tue 18:00 P2

**Structure and thermal Stability of (C60+P2O) and (C60+P4O) Heterolayers on Ag(111)** — •Mohammed Suhail Ansari, Ravi Priya, Keda Jin, and Peter Jakob — Department of Physics, Philipps-Universität Marburg, Germany

This study investigates the interactions between $C_{60}$ fullerene and two organic semiconductors, 6,13-pentacenequinone (P2O) and 5,7,12,14-pentacenetetrone (P4O), on Ag(111) substrates using IRAS, SPA-LEED, and TDS. The aim is to elucidate the structural properties and transformation processes of $C_{60}$ and P2O/P4O under varying preparation conditions and thermal processing. Our findings reveal three different vertical arrangement scenarios of the heterostructures based on the deposition sequence and thermal treatments: (a) Formation of a well-defined bilayer on a pre-deposited monolayer corresponding to the deposition sequence, (b) a complete interlayer exchange of molecules, and (c) a partial interlayer exchange leading to mixed layers. Scenario (a) is observed with a P2O bilayer deposited on a well-defined $C_{60}$ monolayer. Interestingly, P2O adsorbs in an inclined orientation on the $C_{60}$/Ag(111) monolayer. Scenario (b) is observed with deposition of a monolayer of P2O followed by a bilayer of $C_{60}$ at room temperature that results in P2O migration to the second layer, emphasizing the weaker interaction of P2O with the substrate Scenario (c) is found for the combination of $C_{60}$ and P4O and it involves migration of P4O to the second layer if it was deposited in the first layer, and vice-versa. We will discuss in detail the evolution of the grown heterolayers in terms of molecular orientations, interlayer exchange, and intermixing.

O 50.8 Tue 18:00 P2

**Molecular self-assembly of BDA on $CsPbBr_3$(100)** — •Hannah Loh, Andreas Raabgrund, 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. By choosing perticular anchoring groups of organic molecules (here the carboxylic COOH-group) the interaction with the perovskite material may be tuned.

In this contribution we investigate the self assembly of 4-4-biphenyl dicarboxylic acid (BDA) on epitaxial $CsPbBr_3$ on Au(100) [2] by STM. For submonolayer coverage of BDA on $CsPbBr_3$ we find that upon deposition at 305 K molecules grow epitaxially in compact islands. The islands consist of chains with a V-structure inside the chains similar to the way BDA self-assembles on Cu(111) [3].

[1] Bao C. et al., Organic Electronics, **73**, 299-303 (2019)
[2] Rieger J. et al., Phys. Rev. Mat, **7**, 035403 (2023)
[3] Schmitt T. et al., J. Phys. Chem. C, **120(2)**, 1043-1048, (2016)

O 50.9 Tue 18:00 P2

**Structure and charge carrier dynamics of an organic donor/acceptor heterostructure: a LEEM/PEEM study** — •Franz Niklas Knoop, Klaus Stallberg, and Winfried Daum — IEPT, TU Clausthal, Germany

We combine low-energy electron microscopy (LEEM) and two-photon photoemission electron microscopy (2P-PEEM) to study the relation between structure and charge carrier dynamics in well-ordered organic donor/acceptor (D/A) heterostructures of para-sexiphenyl (*p*-6P) and copper-hexadecaphthalocyanine ($F_{16}$CuPc). While *p*-6P monolayers deposited on $SiO_2$ exhibit structural order only on a nanometer scale, *p*-6P islands in the second layer comprise micrometer sized single-crystalline domains. Using microspot low-energy electron diffraction ($\mu$LEED) and dark-field LEEM, on many islands we observe two mirror domains which we attribute to different tilt angles of the *p*-6P molecules in the second layer. Using $\mu$LEED we confirm epitaxial growth of monolayer $F_{16}$CuPc on $SiO_2$/*p*-6P which results in a structurally well-defined organic D/A interface. Especially on *p*-6P bilayer regions, large single-crystalline $F_{16}$CuPc domains are observed. With 2P-PEEM we observe increased photoemission from $SiO_2$/$F_{16}$CuPc after optical pumping at 810 nm. In contrast, for $SiO_2$/*p*-6P/$F_{16}$CuPc the photoemission signal decreases. Also, the reflectivity for low-energy electrons changes upon optical pumping. We relate these long-lived pump-induced effects to intermolecular charge transfer which is more pronounced for bilayer-*p*-6P/$F_{16}$CuPc than for monolayer-*p*-6P/$F_{16}$CuPc.

## O 51: Poster Electronic Structure of Surfaces: Spectroscopy, Surface States

Time: Tuesday 18:00–20:00 Location: P2

O 51.1 Tue 18:00 P2

**Visualizing quantum states in fluorene-based organometallic quantum corrals** — •Longfeng Huang[1], Wenchao Zhao[1], Ignacio Piquero-Zulaica[1], Johannes Barth[1], and Biao Yang[1,2] — [1]Physics Department E20, Technical University of Munich, 85748 Garching, Germany — [2]Institute of Functional Nano and Soft Materials (FUNSOM), Soochow University, 215123 Suzhou, China

Constructing well-defined and controllable quantum states holds promise for applications in quantum technology. As an exemplary quantum architecture, quantum corrals (QCs) which are considered as artificial atoms attract enormous attention.1, 2 Common strategies for manufacturing QCs have mainly involved atomic and molecular manipulations, molecular assembly, and on-surface synthesis.3-5 However, fabricating robust QCs simultaneously with a high yield and specific size still remains elusive. In this work, we realize stable QCs with a well-defined size via organometallic bonding between fluorine-based molecules and intrinsic Ag adatoms on Ag(111). In particular, we observe spatial quantum resonance states inside the QCs, which arise from the scattered two-dimensional electron gas. Additionally, stadium-shaped and triangular QCs exhibit intriguingly specific orbital-like quantum states in differential conductance maps. In addition, we tune the QCs by replacing the F to H atoms and tip manipulation. Our study provides new means to fabricate controllable exotic quantum states with atomically precise QCs, aiding in a rational design strategy towards materials with tailored electronic properties.

O 51.2 Tue 18:00 P2

**Termination-dependent ARPES maps from novel magnetic Kagome metals $GdV_6Sn_6$ and $GdMn_6Sn_6$** — •Robin P. Forster[1], Honey Boban[1], Mohammed Qahosh[1], Xiao Hou[1], Yishui Zhou[2], Yixi Su[2], Claus M. Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum-Jülich — [2]JCNS Forschungszentrum-Jülich

The magnetic Kagome metals $GdV_6Sn_6$ and $GdMn_6Sn_6$ combine in a single material phenomena such as flat Kagome bands [1,2], local moments of the 4f electrons of Gd, and itinerant Mn or V 3d electrons [3], providing a platform to study their complex magentic and electronic interactions. We have performed termination-dependent micro-ARPES measurements with 20 $\mu m$ real-space resolution at 20 K of paramagnetic $GdV_6Sn_6$ [4] and ferrimagnetic $GdMn_6Sn_6$ [5]. Surface and bulk states could be distinguished in the series of scans made over a range of photon energies. We have chosen $h\nu$ of 80 and 130 eV for $GdV_6Sn_6$ and 80, 112, 140, and 200 eV for $GdMn_6Sn_6$ for detailed ARPES scans. In addition, XPS measurements were conducted, which provide an insight into the measured 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] PRB 104, 15122 (2021) [3] JPSJ 90, 124704 (2021) [4] JMMM 202, 519 (1999) [5] PRB 104, 235139 (2021) [6] *arXiv:2410.19652 (2024).

O 51.3 Tue 18:00 P2

**Structural fingerprints in the reflectance anisotropy of P-rich and In-rich AlInP(001)** — •Isaac Azahel Ruiz Alvarado[1], Mohammad Amin Zare Pour[2], Thomas Hannappel[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany — [2]Grundlagen von Energiematerialien, Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The surface optical anisotropy of AlInP(001) surfaces is investigated through experimental and theoretical approaches. Comparison is made between spectra calculated for energetically favored AlInP(001) surface structures with data measured on epitaxially grown Al$_{0.52}$In$_{0.48}$P(001) epilayers lattice-matched to GaAs samples. The anisotropies for photon energies below 3 eV provide clear fingerprints for the structure of the outermost surface atomics layers. The negative anisotropies for P-rich AlInP(001) surfaces are related to transitions involving surface states located at the top P-dimers. In contrast, In-rich AlInP(001) surfaces show anisotropies related to surface states localized on the In atoms of the In dimers of the second row. The spectral features at higher energies provide insight into the near surface bulk ordering of AlInP. In particular, optical anisotropies at the AlInP critical point energies are found to be related to the CuPt ordering in the material.

O 51.4 Tue 18:00 P2

**Next-Gen ARPES: AI-controlled beam polarization through Graphene** — •Ridha Eddhib[1], Balasubramanian Thiagarajan[2], and Jan Minar[1] — [1]New Technologies-Research Centre, University of West Bohemia, 30100 Pilsen, Czech Republic — [2]MAX IV Laboratory, Lund University, Lund, 22100, Sweden

Angle-Resolved Photoemission Spectroscopy (ARPES) stands as a cornerstone technique in condensed matter physics, offering deep insights into electronic structures and quantum states. However, the precision of ARPES measurements critically depends on the exact calibration of the photon beam polarization, a challenge that often confronts experimentalists. This study introduces an innovative application of artificial intelligence (AI) to revolutionize ARPES experiments by enabling precise calibration and tuning of photon beam polarization through graphene ARPES cross section, aiming for the ideal of 100% circular polarization. At the heart of our methodology is a neural network model, meticulously trained on datasets generated by the sophisticated one-step model of the SPRKKR [1] (Spin-Polarized Relativistic Korringa-Kohn-Rostoker) code, renowned for its accurate ARPES simulation capabilities. This study leverages the ase2sprkkr package for streamlined interfacing with SPRKKR, enriching our AI model training data with high-fidelity simulations. By implementing this AI-driven methodology, researchers can dynamically adjust their ARPES setups, ensuring that each measurement is conducted under optimal polarization conditions. [1] Ebert, H., Koedderitzsch, D., & Minar, J. (2011). 74(9), 096501.

O 51.5 Tue 18:00 P2

**The CD-ARPES study of intercalated transition metal dichalcogenide V1/3NbS2** — •Jyoti Kaswan[1], Laurent Nicolaï[1], Raphaël Salazar[1], Aki Ismo Olavi Pulkkinen[1], Sunil W Dsouza[1], Zdeněk Sofer[2], and Jan Minár[1] — [1]University of West Bohemia, Plzeň, Czech Republic — [2]University of chemistry and technology Prague, Czech Republic

Intercalated transition metal dichalcogenides (TMDCs) have recently garnered significant attention from the condensed matter community due to the demonstration of exotic phenomena that depend on the intercalated transition metal [1]. We investigate the electronic structure of V-intercalated TMDC, V1/3NbS2, using Circular Dichroic Angle-Resolved Photoemission Spectroscopy (CD-ARPES) in combination with the one-step model of photoemission as implemented in the SPR-KKR package [2].The intensity asymmetry in CD contains a well-known dichroism component related to the measurement geometry, as well as a component associated with magnetic ordering, complicating the extraction of spin information from CD-ARPES data. To address this challenge, our group has developed a model of dichroism based on the one-step model of photoemission (SPR-KKR code). By incorporating the measurement geometry, the ab initio calculations enable the separation of geometric and spin contributions to the CD signal [3,4]. [1] B. Edwards et al, Nature Materials 22, 459*465 (2023). [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011) [3] O. Fedchenko et al., Sci. Adv. 10, eadj4883 (2024) [4] S. Beaulieu et al, Phys. Rev. Lett. 125, 216404 (2020)

## O 52: New Methods: Experiment

Time: Tuesday 18:00–20:00 Location: P2

O 52.1 Tue 18:00 P2

**Exploring novel scanning force microscopy schemes by stabilising unstable states** — •Lukas Böttcher[1], Hannes Wallner[2], Niklas Kruse[2], Wolfram Just[2], Ingo Barke[1], Jens Starke[2], and Sylvia Speller[1] — [1]Universität Rostock, Institute of Physics — [2]Universität Rostock, Institute of Mathematics

Dynamic scanning Force Microscopy (SFM) is a versatile and popular method for investigation of surface properties on the nanoscale. When probing the surface with an oscillating cantilever bistabilities may occur [1, 2], which are a result of nonlinearities arising due to interaction between tip and sample. By implementing a control scheme, we track the unstable state arising between the two stable states [3]. These unstable states may enable ultra-sensitive imaging conditions and give access to virtually interaction free mapping of material parameters.

[1] Gleyzes, P., Kuo, P.K., Boccara, A.: Bistable behavior of a vibrating tip near a solid surface. Appl. Phys. Lett. 58, 2989 (1991) [2] Misra, S., Dankowicz, H., Paul, M.: 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 et.al, Exposing hidden orbits in scanning force microscopy, in preparation

O 52.2 Tue 18:00 P2

**Surface photovoltage spectroscopy for investigation of SiC surface quality** — •Viktoriia Nikonova[1], Nadine Schüler[1], Steffen Fengler[1], Maaz Soomro[1], Knut Gottfried[2], Imme Ellebrecht[2], and Kay Dornich[1] — [1]Freiberg Instruments GmbH, Delfter Strasse 6, 09599, Freiberg, Germany — [2]ErzM-Technologies UG, Technologie-Campus 1, 09126, Chemnitz, Germany

The surface photovoltage (SPV) technique belongs to the advanced methods for studying charge separation and transfer processes in photoactive materials.

The measurements of the SPV signal amplitude and time constant maps for SiC wafers have been done using a compact HR-SPS tool with fixed energy excitation sources. It has a high flexibility, which for example enables the integration of up to four lasers in the measurement head, either for injection level dependent SPV measurements or extracting depth information by using different wavelengths. Presented method based on fixed capacitor approach, that is much faster and more sensitive than on Kelvin probe. Also it works for highly doped substrate for which microwave based methods are difficult.

The experiments show the difference in maps between surface quality of wafers: polished wafers, fine and coarse grinded surfaces. Thus, the presented technique can be used to make quantitatively based decisions on the goodness of surface treatment methods without damaging the samples and to improve production based on SiC and others wide bandgap materials.

O 52.3 Tue 18:00 P2

**ESEM Automation - Advanced Acquisition & Dual Magnification** — •Maurits Vuijk[1], Annika Kubsch[1], Johannes Zeininger[2], Karsten Reuter[1], Thomas Lunkenbein[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]TU Wien

In Environmental Scanning Electron Microscopy (ESEM) experiments, the acquisition parameters are generally kept constant throughout the collection of the data set. This requires human supervision and limits data collection to one data set at a time. We use a custom automation interface to minimize supervision and allow for the collection of multiple simultaneous data sets containing complementary information.

Slow oscillatory dynamics are observed on a Co surface under hydrogen and oxygen dosing conditions using traditional ESEM. With our automation interface, we can implement more advanced acquisition programs into the microscope that take advantage of different time scales of the surface dynamics. By using automation to change the settings of the acquisition after each frame, we are able to capture multiple interlaced views of the same process. In this case, we alternated between two different magnification values, allowing us to capture a low magnification overview of the propagation of the surface dynamics and a high magnification view of the ongoing local structural changes to a selected surface feature. Many acquisition parameters such as gun voltage, stage position or focus can be automatically adjusted in an intelligent fashion, allowing for more complex acquisition strategies to unravel complex dynamic processes.

O 52.4 Tue 18:00 P2

**Simultaneous Grazing Incidence Small Angle X-Ray Scattering (GISAXS) and Absorption Spectroscopy (XAS) of Liquid Surfaces** — •Carlo Schneider, Lukas Voss, Frederic Braun, and Dirk Lützenkirchen-Hecht — Bergische Universität Wuppertal

A method combining Grazing Incidence Small Angle X-ray Scattering (GISAXS) and X-ray Absorption Spectroscopy (XAS) has been developed to investigate liquid surfaces. The approach employs a specialized reaction cell and detection systems, including a PILATUS 100k detector for scattering data and a PIPS detector for absorption spectra, paired with a Quick EXAFS (QEXAFS) monochromator. Solutions of nickel chloride, cobalt nitrate, and zinc acetate were analyzed to evaluate the feasibility of integrating time-resolved GISAXS with XAS. Results demonstrate the capability of the method to provide structural and compositional information on nanometer and angstrom scales simultaneously. Challenges, such as interference patterns potentially caused by instrumental effects, were identified and suggest areas for further refinement. The developed technique offers potential for applications in materials science and chemistry, enabling insights into liquid systems.

O 52.5 Tue 18:00 P2

**Surface-Sensitive Analysis of Liquid Interfaces: Grazing Incidence X-Ray Absorption Spectroscopy with a Double-Mirror Setup** — •Lukas Voss, Dirk Lützenkirchen-Hecht, Frederic Braun, and Carlo Schneider — Bergische Universität Wuppertal, NRW

Grazing incidence X-ray absorption spectroscopy (GIXAS) is a powerful technique for surface-sensitive investigations. While the study of solid materials can be easily performed by adjusting the sample orientation to vary the X-ray incidence angle, the examination of liquids requires a specialized experimental setup. To address this challenge, a double-mirror system was integrated into an existing reflectometer, enabling GIXAS measurements on liquid samples. This setup was utilized to study the melting behavior of gallium and the formation of sol-gel-derived germanium oxide nanoparticles.

## O 53: Poster Electronic Structure Theory

Time: Tuesday 18:00–20:00 Location: P2

O 53.1 Tue 18:00 P2

**Enhancing Efficiency of Bethe-Salpeter equation calculations including spin-orbit coupling** — •Seokhyun Hong, Cecilia Vona, Sven Lubeck, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin

Calculating optical excitations in materials with significant spin-orbit coupling (SOC) effects is challenging due to the computational costs. We propose a new method to compute optical spectra including excitonic effects within an all-electron framework. This method extends recently introduced second variation with local orbital (SVLO) method[1] towards the Bethe-Salpeter equation (BSE) framework. The SVLO method is based on the conventional second variation (SV) approach for density-funtional theory calculations. In SV, SOC is treated as a perturbation through a two-step procedure. By solving the scalar relativistic (SR) Hamiltonian, we first obtain eigenvalues and states without SOC. A sub-set of these SR Kohn-Sham states is used as basis functions for evaluating the SOC terms. For many materials, this approach can require all available states for convergence and thus may not capture SOC effects accurately without resorting to huge matrix sizes. In the SVLO method, local orbitals (LOs) are included in the SV step as additional basis functions. It could be shown that this enhances the computational efficiency tremendously[1]. Through this work, we have implemented an analogous scheme in the BSE framework. We demonstrate, how we overcome current limitations and achieve highly precise results for materials with strong SOC, such as lead iodide, perovskites, MoS2,etc.

O 53.2 Tue 18:00 P2

**First-Principles Calculations of X-ray Absorption Spectra: Supercell Core-Hole Method versus Bethe-Salpeter Equation** — •Ziyu Wang[1], Lu Qiao[1], Ronaldo Rodrigues Pelá[2], and Claudia Draxl[1] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Zum Großen Windkanal 2, 12489 Berlin, Germany — [2]Supercomputing Department, Zuse Institute Berlin (ZIB), Berlin, Takustraße 7, 14195 Berlin, Germany

Accurate simulations of X-ray absorption spectra (XAS) are essential for understanding core-level excitations and electronic structure. In this study, we compare two approaches for calculating XAS: the supercell core-hole (SCH) method based on density-functional theory and the Bethe-Salpeter equation (BSE) of many-body perturbation theory. In the SCH method, core excitations are simulated by removing a core electron from the system, thus treating electron-hole interaction on the DFT level. In contrast, excitonic effects are considered explicitly in the two-body Hamiltonian underlying the BSE. We apply the SCH method with various exchange-correlation (xc) functionals of DFT to calculate XAS in diverse materials (metals, semiconductors, and insulators) and absorption edges. By comparing them with XAS obtained from BSE, we evaluate in which cases the SCH method is appropriate to be applied.

## O 54: Poster New Methods: Theory

Time: Tuesday 18:00–20:00 Location: P2

O 54.1 Tue 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

In the last decade, Machine Learning Potentials (MLPs) have become an established tool for describing potential energy surfaces (PESs) 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 and it is of high interest to reduce the number of structures to be computed as well as their complexity. 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 55: Poster Topology and Symmetry-protected Materials

Time: Tuesday 18:00–20:00 Location: P2

O 55.1 Tue 18:00 P2

**Native $Bi_2Se_3$ bulk and surface defects calculated from first principles** — •Juntao Kong[1], Timur Biktagirov[2], Uwe Gerstmann[3], and Wolf Gero Schmidt[4] — [1]Warburger Str. 100,33098 Paderborn,Germany — [2]Warburger Str. 100,33098 Paderborn,Germany — [3]Warburger Str. 100,33098 Paderborn,Germany — [4]Warburger Str. 100,33098 Paderborn,Germany

$Bi_2Se_3$ attracts great attention presently because it is a strong topological insulator with its surface state consisting of a single Dirac cone at $\Gamma$ which is protected by timereversal symmetry. Defects in the bulk, such as selenium vacancies, may introduce charge carriers that interfere with these surface states and reduce the ability to isolate surface conduction, which is critical for applications in quantum computing and spintronic devices. Surface defects, on the other hand, may act as active sites for adsorbing gas molecules, enabling changes in electronic properties that can be used for gas sensing. Here, we present a first principles study of native point defects in $Bi_2Se_3$. In particular, the formation energies of vacancies, antisites and interstitials [1,2] are investigated in dependence on Fermi level position and preparation conditions.

O 55.2 Tue 18:00 P2

**Exploring magnetism, topology, and magnetoresistance in rare-earth based compound GdAuSn: Ab initio study** — •Sumit Mondal[1], Japsreet Singh[2], and Kanachana Venkatakrishnan[2] — [1]Central University of Haryana — [2]Indian Institute of Technology, Hyderabad

Among rare-earth intermetallics, Gd-based compounds have garnered particular interest due to their diverse magnetic ground states and interesting non-trivial topological properties. In the present work, we investigate the magnetic, electronic, and dynamical properties of the equiatomic ternary compound GdAuSn using first-principles calculations. We explore its crystal structure and analyse various magnetic configurations to determine the ground state. Our results indicate that the C-type antiferromagnetic configuration has the lowest energy. By correlating the spin configurations with the underlying Heisenberg spin model, we determine the exchange interactions and calculate the critical tempera- ture using the mean-field approximation. Additionally, we examine the electronic band structure and find evidences of nodal surface and Dirac points, indicative of non-trivial topology. Furthermore, we analyse the longitudinal and transverse magnetoresistance behaviour of GdAuSn under varying magnetic fields, observing intriguing trends that suggest a correlation between magnetic field strength and magnetoresistance. Finally, we assess the phonon dispersion of our compound and find the topological phononic states with nodal surfaces. Our findings shed light on the magnetism, topology, and transport properties in rare-earth-based intermetallic compound.

O 55.3 Tue 18:00 P2

**Graphene intercalation of the large gap quantum spin Hall insulator bismuthene** — •Lukas Gehrig[1,2], Cedric Schmitt[1,2], Bing Liu[1,2], Jonas Erhardt[1,2], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany

Bismuthene, a honeycomb monolayer of bismuth atoms synthesized on a SiC(0001) substrate, is a topological insulator with a breakthrough bulk band gap of 800 meV due to giant spin-orbit coupling. The magnitude of this gap exposes bismuthene as a promising candidate for room temperature spintronic applications based on the quantum spin Hall effect. However, oxidation of bismuthene in air confines most experiments on this system to UHV conditions. Here we demonstrate the intercalation of bismuthene between SiC and a single sheet of graphene. This protective layer effectively prevents bismuthene from oxidation, while it fully conserves its structural and topological properties as we readily demonstrate by scanning tunneling microscopy and photoemission spectroscopy. This paves the way for ex-situ experiments and ultimately brings bismuthene closer to the fabrication of spintronic devices.

# O 56: Overview Talk Pavel Jelinek

Time: Wednesday 9:30–10:15 Location: H24

**Topical Talk** O 56.1 Wed 9:30 H24

**trends and perspectives in on-surfece UHV synthesis** — •Pavel Jelínek — Institute of Physics of the Czech Academy of Sciences, Cukrovarnicka 10, Prague 6, Czechia

On-surface synthesis in ultra-high vacuum conditions has demonstrated the capability to synthesize molecular structures that are not available through traditional methods in solutions [1]. For example, the synthesis of radical PAH molecules on metal surfaces and their subsequent characterization with the help of UHV SPM contributed significantly to the progress in pi-magnetism [2]. In this talk, we will discuss the current status and perspectives of the field. We will also review what makes the on-surface synthesis on metallic surfaces unique concerning synthesis in solution. This includes the 2D constraint imposed by the proximity of the surface as well as the essential catalytic role of single atoms diffusing on metal surfaces [3], so-called adatoms, at elevated temperatures has been pointed out [4].

[1] S. Clair and D. G. de Otyeza Chem. Rev. 119, 4717 (2019); L. Grill et al, Nature Nano 2, 687 (2007). [2] D.G. de Otyeza and T. Frederiksen JPCM 34, 443001 (2022). [3] H. Brune, Surf. Sci. Rep. 31, 125 (1998). [4] J.I. Mendieta-Moreno et al, Angew. Chem. Int. Ed. 61 e202208010 (2022).

# O 57: Ultrafast Electron Dynamics I

Time: Wednesday 10:30–13:00 Location: H2

O 57.1 Wed 10:30 H2

**Imaging the subcycle dynamics of topological surface currents in two-dimensional momentum space** — •Tim Bergmeier[1], Suguru Ito[1], Jens Güdde[1], and Ulrich Höfer[1,2] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Fachbereich Physik, Universität Regensburg, Germany

Angle-resolved photoemission spectroscopy (ARPES), combined with THz-electric fields and subcycle temporal resolution, offers unique capabilites to explore light-matter interaction on timescales faster than the oscillation of a lightwave. With this approach, it is possible to directly observe the dynamics of lateral Dirac currents along the surface of topological insulators, as well as the ultrafast buildup and dephasing of Floquet-Bloch states. However, so far the momentum resolution of such experiments was restricted to only 1-dimensional cuts within the surface momentum space.

Here, we present first results on the subcycle dynamics of surface currents resolving the full Dirac cone of $Bi_2Te_3$. In our recently established setup in Marburg, a 200 kHz laser system allows for MV/cm field strengths by parametric amplification of frequency-tunable THz-pulses in the range of 20-40 THz, together with optimal focussing at large angles of incidence inside of the UHV chamber by astigmatism compensation. Combined with ultrashort 400nm two-photon probe pulses (<15 fs) and a Scienta DA30 photoelectron analyzer, we are able to measure the whole 2D-momentum space with subcycle resolution.

O 57.2 Wed 10:45 H2

**Measuring the non-equilibrium electronic structure of phonon-driven 2D materials** — •Niklas Hofmann and Isabella Gierz — University of Regensburg

Quasi-periodic driving of solids with tailored light fields has emerged as a promising pathway for non-equilibrium materials design. To bring this approach to the next level, tailored driving schemes targeting specific degrees of freedom need to be combined with ultrafast probes of the atomic and electronic structure. We combine pump pulses tunable all the way from the Terahertz to the visible spectral range with a time- and angle-resolved photoemission (trARPES) probe to gain access to the transient electronic structure of driven materials. We recently implemented a narrow-band, strong-field Terahertz source [1] that allows for the selective excitation of phonon modes in materials with strong spin-orbit coupling and extreme ultraviolet probe pulses with tunable pulse duration to trace band structure dynamics on sub-cycle as well as cycle-averaged time scales. In this talk we present proof-of-principle experiments on graphene and show the transient electronic structure of $WS_2$ driven at resonance to the $E_{1u}$ phonon mode.

[1] Optics Letters 42, 129 (2017)

**Invited Talk** O 57.3 Wed 11:00 H2

**Floquet engineering in black phosphorus** — •Changhua Bao[1,2], Shaohua Zhou[2], Benshu Fan[2], Michael Schüler[3], Teng Xiao[2], Hui Zhou[4], Zhiyuan Sun[2], Peizhe Tang[5], Sheng Meng[4], Wenhui Duan[2], and Shuyun Zhou[2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Physics, Tsinghua University, Beijing, China — [3]Laboratory for Materials Simulations, Paul Scherrer Institute, Switzerland — [4]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [5]School of Materials Science and Engineering, Beihang University, Beijing, China

The time-periodic light field has emerged as a control knob for manipulating quantum states in solid-state materials, dubbed as Floquet engineering. In this talk, I will present our progress on the experimental realization of Floquet band engineering in a model semiconductor, black phosphorus. Driven by strong mid-infrared light fields, transient gap opening and band renormalization are directly resolved with exotic pseudospin selectivity. In addition to band-structure engineering, manipulation of symmetry properties through Floquet engineering is also explored, including ultrafast glide-mirror symmetry breaking and parity symmetry manipulation. This series of works provides a comprehensive understanding of Floquet engineering in semiconductors and important guidance for extending Floquet engineering into more materials.

Nat. Rev. Phys. 4, 33 (2022); Nature 614, 75 (2023); PRL 131, 116401 (2023); ACS Nano 18, 32038 (2024); Nat. Commun. in press

O 57.4 Wed 11:30 H2

**Observation of Floquet states in graphene** — •Marco Merboldt[1], Michael Schüler[2], David Schmitt[1], Jan Philipp Bange[1], Wiebke Bennecke[1], Karun Gadge[3], Salvatore R. Manmana[3], Sabine Steil[1], G. S. Matthijs Jansen[1], Daniel Steil[1], Michael Sentef[4], Marcel Reutzel[1], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany — [2]Department of Physics, University of Fribourg, Fribourg, Switzerland — [3]Georg-August-Universität Göttingen, Institut für Theoretische Physik, Germany — [4]Institute for Theoretical Physics, University of Bremen, Bremen, Germany

Recent advances in the field of condensed-matter physics have unlocked the potential to realize and control emergent material phases that do not exist in thermal equilibrium. One of the most promising concepts in this regard is Floquet engineering, the coherent dressing of matter via time-periodic perturbations. However, the broad applicability of Floquet engineering to quantum materials is in question, especially with respect to (semi-)metals and graphene in particular.

Here, we resolve this long-standing debate by using electronic structure measurements to provide direct spectroscopic evidence of Floquet effects in graphene [1]. We report light-matter-dressed Dirac bands by measuring the contribution of Floquet sidebands, Volkov sidebands, and their quantum path interference to graphene's photoemission spectrum. Fully supported by experiment and theory, we demonstrate that Floquet engineering in graphene is possible.

[1] Merboldt *et al.*, arXiv:2404.12791 (2024)

O 57.5 Wed 11:45 H2

**Theory of nonperturbative nonlinear transport in a Floquet-Weyl semimetal** — •Juan Ignacio Aranzadi[1], Matthew Day[2,3], James McIver[2,3], and Michael Sentef[1,2] — [1]Institute for Theoretical Physics, University of Bremen/ Bremen Center for Computational Material Science, Bremen — [2]Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg — [3]Department of Physics, Columbia University, New York, NY, USA

Weyl semimetals exhibit unique topological properties characterized by pairs of Weyl nodes with opposite chirality. While their transport properties have been extensively studied [1], their behavior under strong optical driving fields remains poorly understood. In this regime, the material response is governed by photon-dressed Floquet-Bloch states. Here, we investigate the photocurrent production mechanisms in Td-MoTe2, a type-II Weyl semimetal, under strong circularly polarized fields. Recent transport measurements in this material revealed a linear scaling of photocurrents at strong fields (<0.4 MV/cm) for the circular photogalvanic effect and the light-induced Hall effect [2]. We explore the microscopic theory underlying the photocurrent production in this system and disentangle its various contributing mechanisms. [1] J. Hu, S. Xu, N. Ni, Z. Mao, Annual Review of Materials Research (2019) 49:1, 207-252 [2] M. Day et. al. Nonperturbative nonlinear transport in a topological light-matter hybrid (2024)

O 57.6 Wed 12:00 H2

### 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.*, arXiv:2411.14993 (2024)

O 57.7 Wed 12:15 H2

### Characterization of Excitons for bulk Black Phosphorus

— •Juan Felipe Pulgarin Mosquera[1,2], Geoffroy Kremer[2,3], Claude Monney[2], and Michael Schueler[1,2] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]Department of Physics, University of Fribourg, CH-1700 Fribourg, Switzerland — [3]Institut Jean Lamour, CNRS-Université de Lorraine

Excitons (coupled electron-hole pairs) in semiconductors can form collective states that exhibit spectacular nonlinear properties and possible applications in future optoelectronic devices. We present here some theoretical methods and a workflow for determining the excitonic wave functions and the corresponding excitonic binding energies for bulk Black Phosphorus. We solve the Bethe-Salpeter equations for coherent and incoherent excitations. The theoretical/numerical results are compared to the experimental ones of angle resolved photoemission spectroscopy (ARPES), by analyzing the spectra produced after including non-equilibrium electron-phonon dynamics; solving the time-dependent Boltzmann equation. These results allow us to understand the nature and characteristics of these two-particle bound states, together with some scattering effects, being challenging due to the stronger screened potential for 3D materials, resulting in short time excitations.

O 57.8 Wed 12:30 H2

### Momentum-resolved valleytronic dynamics in TMDC monolayers

— •Sarah Zajusch[1], Lasse Münster[2], Marcel Theilen[1], Marleen Axt[1], Yaroslav Gerasimenko[2], Jens Güdde[1], Robert Wallauer[1], and Ulrich Höfer[1,2] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]Fachbereich Physik, Universität Regensburg

The lack of inversion symmetry allows to access the valley degree of freedom in TMDC materials. With circular polarized light, time-resolved momentum microscopy enables us to trace the formation of a rich variety of bright and dark excitons typical for these materials on an ultrafast timescale and throughout the whole Brillouin zone.

We performed measurements on both MoSe$_2$ and WS$_2$. In WS$_2$, we observe a valley depolarization at room temperature within 100 fs, whereas in MoSe$_2$, this happens on a slower timescale, with a slight polarization that is still visible long after 100 fs. There are mainly two proposed leading mechanisms for this relaxation process, exciton-phonon scattering and electron-hole exchange interaction, which are differently pronounced in W- and Mo-based TMDCs due to the differences in their excitonic energy landscapes. As the ultrafast formation of dark KK'- and KΣ-excitons in WS$_2$ shows, mainly exciton-phonon scattering contributes to the valley relaxation here. This process is strongly temperature-dependent.

O 57.9 Wed 12:45 H2

### Formation and thermalization of non-equilibrium excitonic occupations

— •Paul Werner[1], Jan P. Bange[1], Wiebke Bennecke[1], Giuseppe Meneghini[2], David Schmitt[1], Marco Merboldt[1], Anna Seiler[1], AbdulAziz AlMutairi[3], Samuel Brem[2], Junde Liu[1], Daniel Steil[1], Stephan Hofmann[3], R. Thomas Weitz[1], Ermin Malic[2], Stefan Mathias[1], and Marcel Reutzel[1] — [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

Semiconducting transition metal dichalcogenides (TMDs) host a rich landscape of Coulomb-correlated electron-hole pairs, which makes them ideal candidates for future optoelectronic applications. After an initial optical excitation of bright excitons, it is known that subsequent scattering into optically dark excitons takes place [1]. However, these processes must involve non-thermal exciton distributions that thermalize to a quasi-equilibrium [2]. In this work we use time-resolved momentum microscopy to directly access these non-thermal exciton distributions in optically excited homobilayer MoS$_2$. We identify the exciton landscape and relaxation pathways, and we find clear signatures of the non-equilibrium exciton distributions that are involved in the thermalization process. We compare our data with a full microscopic model calculation that confirms our experimental findings.

[1] Bange *et al.*, 2D Materials **10** 035039 (2023)

[2] Rosati *et al.*, ACS Photonics **7**, 2756–2764 (2020)

# O 58: Solid-Liquid Interfaces: Reactions and Electrochemistry II

Time: Wednesday 10:30–13:00 Location: H4

O 58.1 Wed 10:30 H4

**Step Bunching Instability and its Effects in Electrocatalysis on Platinum Surfaces** — •Francesc Valls Mascaró[1], Marc T. M. Koper[2], and Marcel J. Rost[3] — [1]Departement of Physical Chemistry, University of Innsbruck — [2]Leiden Institute of Chemistry, Leiden University — [3]Huygens-Kamerlingh Onnes Laboratory, Leiden Institute of Physics, Leiden University

The atomic-scale surface structure plays a major role in the electrochemical behaviour of a catalyst. The electrocatalytic activity towards many relevant reactions, such as the oxygen reduction reaction on platinum, exhibits a linear dependency with the number of steps until this linear scaling breaks down at high step densities. In this work we show, using Pt(111)-vicinal surfaces and in situ electrochemical scanning tunnelling microscopy, that this anomalous behaviour at high step densities has a structural origin and is attributed to the bunching of closely spaced steps. While Pt(554) presents parallel single steps and terrace widths that correspond to its nominal, expected value, most steps on Pt(553) are bunched. Our findings challenge the common assumption in electrochemistry that all stepped surfaces are composed of homogeneously spaced steps of monoatomic height and can successfully explain the anomalous trends documented in the literature linking step density to both activity and potential of zero total charge [1].

[1] F. Valls Mascaró, M. T. M. Koper, and M. J. Rost, Nat. Catal. 7, 1165 (2024)

O 58.2 Wed 10:45 H4

**ALD coatings on 1D and 3D structures for electrochemical applications** — •Siow Woon Ng — Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Atomic layer deposition (ALD) utilizes self-limiting surface reactions to construct ultrathin films layer by layer. Among many deposition techniques, ALD uniquely offers conformal deposition and excellent coating thickness control. Hence, the technique is particularly attractive for depositing structures with complex geometries, such as spheres, foams, 1D nanostructures, and 3D structures. This presentation discusses the preparation of 1D nanostructure and 3D-printed structures, followed by ALD inorganic and semiconductor coatings on these scaffolds. The influence of surface properties on the ALD coatings, and how the coatings enhance the electrical, mechanical, optical, and chemical properties or introduce new functionalities to the host structures will be presented. In particular, we will demonstrate that thin coatings in nanometer thicknesses are optimized for sensing and photo- and electrocatalytic applications.

O 58.3 Wed 11:00 H4

**echemdb - a Database for Electrochemical and -catalytic Data of Metal Single-Crystal Electrodes** — •Johannes Hermann[1], Julian Rüth[2], Nicolas G. Hörmann[3], Nicolas Bergmann[3], Karsten Reuter[3], Timo Jacob[1], and Albert K. Engstfeld[1] — [1]Institute of Electrochemistry, Ulm, DE — [2]Julian Rüth GmbH, DE — [3]Fritz-Haber-Institut der MPG, Berlin, DE

Over the last decades and still today, electrochemical and catalytic studies on metal single-crystal electrodes form the basis of our fundamental understanding of atomic-scale processes on such electrodes and more complex catalyst materials, such as supported nanoparticles, found in applications. So far, experimental data and information on the data are mostly only available as traces and plain text in published works, which limits the FAIR (findable, accessible, interoperable, and reusable) use of the data in further experimental and theoretical works. To mitigate this issue, we present an open-source community approach to store such data and metadata in a structured way in a dedicated database, using the frictionless framework combined with a simple metadata standard. We illustrate the challenges associated with setting up such a system for the underlying data types, highlight tools that allow recovering data from published works and storing new data from experimental and theoretical works similarly. We demonstrate that these tools are equally applicable to other research areas. Finally, we provide some examples of using such a database in daily routines (finding and comparing experimental and theoretical data) and system-specific studies (reusability).

O 58.4 Wed 11:15 H4

**The direct comparison of Pt and Cu particles on a $TiO_2$ photocatalyst in the hydrogen evolution reaction** — •Lucia Mengel[1], Pieter van den Berg[2], Martin Tschurl[1], Neill Goosen[2], 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]Department of Process Engineering, Stellenbosch University, Banghoek Rd, Stellenbosch Central, Stellenbosch, 7599, South Africa

Anatase $TiO_2$ loaded with a metal co-catalyst is a well-known photocatalyst for hydrogen evolution. Fundamental studies on this system often employ photoreforming of alcohols as model reaction, utilizing noble metals such as platinum as a co-catalyst. The hole-mediated photooxidation reaction of the alcohol yields hydrogen next to valuable organic compounds such as aldehydes. Recent efforts aim at a replacement of platinum as co-catalyst by the more abundant and less expensive copper. In our work, we focus on the evolution of hydrogen on copper-loaded anatase by performing ethanol photoreforming in the liquid phase in oxygen- and water-free conditions. We study the hydrogen evolution reaction under excitation with UV-light and compare the photoactivity of the system to a common platinum-loaded catalyst and discuss possible scenarios for the interpretation of the reaction behavior.

O 58.5 Wed 11:30 H4

**Microkinetic Modeling of the Hydrogen Evolution Reaction in Alkaline Conditions** — •Dipam Patel and Georg Kastlunger — Technical University of Denmark

The Hydrogen Evolution Reaction (HER) in alkaline media is distinguished from the acidic case by the source of H. Significant theoretical work has investigated and diagnosed activity in acidic conditions, but this understanding does not necessarily correspond to alkaline. The implications of the stronger O-H bond in H2O compared to that in H3O+ are not yet fully understood. Using constant-potential electrochemical barriers, we developed a microkinetic model of alkaline HER activity on a selection of close-packed metallic surfaces. By accounting for the different potential responses of catalysts, we are able to reproduce the relative rates and tafel slopes seen in experiment. By relating the calculated activities to electrochemical descriptors, we show that the application of solely hydrogen binding descriptors, as in acidic HER, does not fully explain HER activity in alkaline.

O 58.6 Wed 11:45 H4

**Predicting Charge Effects at 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]Laboratory of Theory and Simulation of Materials, EPFL, Lausanne

Computational modeling of electrified solid-liquid interfaces must account for capacitive contributions at potentials beyond the point of zero charge (PZC) [1]. These contributions can approximately be obtained from first-principles calculations at constant charge, employing a second-order Taylor expansion that involves the surface's free energy, the work function, and the interfacial capacitance at the PZC [2]. Machine learning (ML) surrogate models have already successfully been employed to predict the PZC energies at significantly reduced computational costs. Here, we extend this by presenting a ML model for work functions and apply this to two standard electrode modeling setups. By including the derivatives of the atomic forces with charge, we stabilize our model and predict the atomic effective charge. As an outlook, we show how this methodology could be utilized to run molecular dynamics simulations at charged conditions and electrochemical barrier calculations.

[1] N. Bergmann, N.G. Hörmann, and K. Reuter, J. Chem. Theory Comput. **19**, 8815 (2023).

[2] N.G. Hörmann and K. Reuter, J. Chem. Theory Comput. **17**, 1782 (2021).

O 58.7 Wed 12:00 H4

**Dynamics at metal-water interfaces for catalytic hydrogenation** — Tien Le[1], Shoutian Sun[1], and •Bin Wang[1,2] — [1]University of Oklahoma, Norman, Oklahoma, US — [2]Max Planck Institute for

Sustainable Materials GmbH, Düsseldorf, Germany

The presence of water has been shown to enhance hydrogenation of polar chemical functional groups, such as C=O and N=O bonds, through proton shuttling. To demonstrate such rather sophisticated reaction pathways, explicit solvent models with dynamic change of local solvent structures should be considered. Beyond what we reported previously for water-promoted C=O hydrogenation in furfural, in this presentation, we will highlight how the dynamics of the local water structures within the first solvation shell may affect the hydrogenation kinetics. Specifically, we find that the activation barriers correlate well with some collective variables that determine the local configuration and relative positions of surface hydrogen and water. We further show that such dynamics of the metal-water interfaces can be manipulated by different approaches to tune the reaction kinetics. Our findings thus provide fundamental insights of this dynamic transformation at the solid-liquid interface and its impact on catalytic activity and selectivity.

O 58.8 Wed 12:15 H4

**Rough Choice: Comparing 1- and 2D Representations of Electrocatalyst Morphology in Multiscale Models** — •Hemanth S. Pillai, Hendrik H. Heenen, Karsten Reuter, and Vanessa J. Bukas — Fritz Haber Institute der MPG, Berlin

While electrocatalyst morphology is often used to tune product selectivity in electrochemical systems, the precise mechanism underpinning this relationship still remains elusive. Recently, we highlighted the role of morphology impacting product selectivity through a "Desorption–Re-adsorption–Reaction" mechanism [*Nat. Catal.* 7, 847*854 (2024)]. In particular, the catalyst morphology steers the competition between two elementary steps: either the desorption and diffusion of an intermediary byproduct or its re-adsorption and further reaction. Within such a model, morphology is captured in an effective manner via a surface roughness descriptor, however some systems may require a more explicit representation of the catalyst morphology. To assess this we employ a transport coupled kinetic model and systematically improve the representation of the catalyst from an effective one-dimensional descriptor to an explicit two-dimensional catalyst morphology. We find that deviations between the two descriptions are governed by morphological and transport parameters, i.e. diffusion length, particle size, shape, and interparticle distance. To conclude, we demonstrate that detailed morphological descriptions are only necessary within a narrow parameter window, thus providing guidance for selecting appropriate representations.

O 58.9 Wed 12:30 H4

**Atomistic Simulation of Platinum-Water Interface: Deep Potential Molecular Dynamics (DP-MD)** — •Muhammad Saleh[1], Alexander Lozovoi[2], Riccardo Martina[1], Matthew Darby[2], Clotilde Cucinotta[2], and Marialore Sulpizi[1] — [1]Theoretical Physics of electrified liquid-solid interface, Ruhr-University Bochum, Germany — [2]Department of Chemistry, Imperial College London, UK

The interaction between platinum surfaces and water holds significant importance due to its extensive applications in catalysis and electrochemical reactions. However, investigating these interactions at the atomistic level presents considerable experimental challenges. Moreover, accurately modeling such systems demands a substantial number of atoms (exceeding 1000), which can impede computational efficiency, particularly when using high-quality methods. In this study, we utilize the capabilities of machine learning potentials, specifically Deep Potential Molecular Dynamics (DP-MD), to overcome these challenges and achieve comprehensive simulation trajectories. This approach allows for an in-depth analysis, providing valuable insights into the surface properties.

O 58.10 Wed 12:45 H4

**Preparation and Electrochemical Characterization of Metal Bicrystal Electrodes** — •Nadine Wölfel, Albert K. Engstfeld, and Timo Jacob — Institute of Electrochemistry, Ulm, DE

The activity of a metal-based electrocatalyst strongly depends on its structural properties, where grain boundaries (GB) can play a significant role. One approach to study the impact of GBs is by varying the grain size of a material, which changes the GB density. In our study we aim at gaining fundamental insights into the atomic scale electrochemical and -catalytic processes at a GB, separating two surfaces with specific crystallographic orientation. We demonstrate how such electrodes can be prepared from Pt wires using the controlled atmosphere flame fusion method [1]. Here, poly-oriented single crystals are formed from two wires, crystallizing as a poly-oriented bicrystal from a common melt. By carefully polishing the poly-oriented crystal along the surface orientation of interest, a planar bicrystal surface with a single GB can be created. The structural properties of the prepared electrodes are determined by Laue X-ray diffraction, scanning electron microscopy (SEM), and electron backscatter diffraction (EBSD) spectroscopy. Electrochemical measurements, such as cyclic voltammetry (CV) are presented, which, based on the features in the CV, provide insights into the available facets and defects. The local electrocatalytic activity of the GB can be elucidated by scanning electrochemical microscopy (SECM) measurements.

[1] FM Schuett et al., Angewandte Chemie, 132 (2020) 13348-13354

## O 59: Spins on Surfaces at the Atomic Scale I

Time: Wednesday 10:30–13:00 Location: H6

O 59.1 Wed 10:30 H6

**Quantum spin engineering in bottom-up assembled molecular nanostructures** — •Taner Esat[1,2], Dmitriy Borodin[3,4], Jeongmin Oh[1,2], Andreas Heinrich[3,4], Stefan Tautz[1,2,5], Yujeong Bae[3,4], and Ruslan Temirov[1,2,6] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance, Germany — [3]Center for Quantum Nanoscience, Institute for Basic Science, South Korea — [4]Ewha Womans University, South Korea — [5]RWTH Aachen University, Germany — [6]University of Cologne, Germany

Scanning tunneling microscopy (STM) is a powerful technique for fabricating and studying artificial nanostructures with purpose-engineered quantum states. Using the manipulation capabilities of the STM, we place aromatic molecules in an upright geometry on a pedestal of two transition metal atoms on the surface [1] and on the STM tip. These nanostructures carry electron spins that are well decoupled from the metallic substrate [2]. Based on this, we fabricate a single-molecule quantum sensor at the apex of the STM tip and address it by electron spin resonance. We use this sensor to measure the magnetic and electric dipole fields emanating from a single atom with sub-angstrom spatial resolution [3]. Finally, we show that varying the transition metal atoms in the pedestal alters the spin state of the molecular nanostructures, leading to exceptionally long spin lifetimes of up to several minutes. [1] Esat et al., Nature 558, 573 (2018) [2] Esat et al., Phys. Rev. Research 5, 033200 (2023) [3] Esat et al., Nat. Nanotechnol. 19, 1466 (2024)

O 59.2 Wed 10:45 H6

**Tuning the Kondo temperature of Porphyrin molecules via adsorption configurations.** — •Xiangzhi Meng[1], Jenny Möller[2], Rodrigo Menchón[3], Alexander Weismann[1], Daniel Sánchez-Portal[3], Aran Garcia-Lekue[3], Rainer Herges[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, 24098 Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität, 24098 Kiel, Germany — [3]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastián, Spain

Magnetic molecules may serve as building blocks for spintronic devices at the ultimate limit of miniaturization. This sort of application requires an understanding of their spin properties. An important example is the Kondo effect that originates from the exchange interaction between a localized magnetic moment and the conduction electrons of the host metal. The interaction strength is reflected by a characteristic temperature, the Kondo temperature TK. In this work, we will show the Kondo effect of cobalt(II)-5,15-bis(4'-bromophenyl)-10,20-bis(4'-iodophenyl)porphyrin (CoTPPBr2I2) molecules on an Au(111) surface with a low-temperature STM. In comparison with the molecules reported before, the Kondo temperature of CoTPPBr2I2 can be tuned over a much broader range (8 K to 250 K) by switching their configurations. Additionally, we show that surface reconstruction plays a crucial role in modulating the molecular Kondo effect.

O 59.3 Wed 11:00 H6

**Fock-Darwin states in tunable artificial atoms with high spin-orbit coupling** — •Julian H. Strik, Hermann Osterhage, Kira Junghans, Niels P.E. van Mullekom, Emil Sierda, Anna M.H. Krieg, Danis Badrtdinov, Daniel Wegner, Mikhail I. Katsnelson, Malte Rösner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

Quantum simulators are a pathway to study novel physical phenomena which are difficult to predict or observe in synthesized materials. To date, there is still a lack of viable platforms for quantum simulation to study confined electrons in strong magnetic fields, namely in the limit that the magnetic length is on the order of the Bohr radius. For typical crystals, this corresponds to field strengths that are unattainable in a laboratory.

In this talk I will discuss the magnetic response of atomic-scale quantum dots based on individual Cs atoms on the semiconducting surface of InSb [1]. Using low-temperature scanning tunnelling microscopy and spectroscopy, we pattern quantum dots of various sizes and geometries, by sculpting the potential of the underlying 2DEG. We then study the LDOS of these various structures to an external magnetic field. We relate this to the Fock-Darwin model of atomic states [2]. We review the experimental results in this context and discuss the role of structure size, symmetry and spin-orbit coupling.

[1] E. Sierda, et al, Science 380, 1048 (2023).
[2] L. P. Kouwenhoven et al., Rep. Prog. Phys. 64, 6 (2001).

O 59.4 Wed 11:15 H6

**Nickelocene-functionalized tips as a molecular spin sensor** — •Diego Soler-Polo[1], Ana Barragán[2], Andrés Pinar Solé[1], Manish Kumar[1], Oleksandr Stetsovych[1], Ben Lowe[1], Elena Pérez-Elvira[2], Koen Lauwaet[2], Pavel Jelínek[2], and José Ignacio Urgel[2] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [2]IMDEA Nanoscience, Cantoblanco, Madrid, Spain

Polyradicals nanographenes with low-lying spin excitations have almost degenerate states with different spins. Even Many-Body methods such as CASSCF and NEVPT2 might not provide enough accuracy to determine the spin of the real ground state. Here, we demonstrate that scanning probe microscopy with a nickelocene-functionalized tip can distinguish between nearly degenerate spin states of single molecular $\pi$-magnets. The nickelocene molecule has a spin 1 and a small magnetic anisotropy of 4 meV that interacts with the molecular spins of the sample. The spectroscopic patterns as we the tip is approached can be related to the number of radicals and their couplings. Such patterns are well reproduced by simple spin models and the corresponding simulated inelastic current. First, the molecular radicals are fitted to a spin hamiltonian, which is then coupled to the S=1 modelling the nickelocene. A cotunneling formalism adapted to spin hamiltonians provides the dIdV maps comparable with the experimental measurements, thus revealing the spin of the sampled system.

O 59.5 Wed 11:30 H6

**Vibrational excitations in magnetic triangular nanographenes** — Nils Krane[1], •Elia Turco[1], Annika Bernhardt[2], Michal Juríček[2], Roman Fasel[1,3], and Pascal Ruffieux[1] — [1]Empa - nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland — [2]University of Zurich, Zurich, Switzerland — [3]University of Bern, Bern, Switzerland

Inelastic electron tunneling spectroscopy has become a powerful tool for the investigation of excited states in single molecules and other quantum dot systems. These excited states can be of various origins, notably from higher energy spin states but also from vibrational modes. Especially in the case of carbon-based molecules, featuring $\pi$-magnetism with strong exchange coupling, both excitation mechanisms can be found within one system. Here, we present a simple method to distinguish between these two mechanisms by spatial mapping of the excited states without any need for high magnetic fields. As a model system, we investigate the spin $S = 1/2$ phenalenyl radical on Au(111) and observe the featuring of two excited states via inelastic tun-neling spectroscopy. Comparison with DFT calculations proofs the vibrational origin of the observed inelastic features and allows us to assign them to distinct vibrational modes.

O 59.6 Wed 11:45 H6

**Realization of separation of time scales in a heterogeneous atomic Boltzmann machine** — •Kira Junghans, Hermann Osterhage, Werner M. J. van Weerdenburg, Niek M. M. Aarts, Anna M. H. Krieg, Tren Jacobs, Niels P. E. van Mullekom, Ruben Christianen, Eduardo J. Domínguez Vázquez, Hilbert J. Kappen, and Alexander A. Khajetoorians — Radboud University, Nijmegen, The Netherlands

The Boltzmann machine (BM) describes an energy-based neural network formed by coupled, fluctuating Ising spins [1]. A material realization of the Boltzmann machine was constructed using the complex stochastic dynamics of coupled Co atoms on the surface of black phosphorus (BP) [1]. Neurons and synapses were realized by a separation of time scales exploiting the anisotropic electronic structure of BP [1]. Using the anisotropy of the substrate is a limitation in scaling this concept.

Here, we study the coupled dynamics of different types of atoms on BP, which exhibit orbital memory [2,3]. We study the influence of the coupling on stochastic dynamics in heteroatomic dimer and trimer configurations with scanning tunneling microscopy (STM). Further, we discuss how the multi-well energy landscape can be influenced by an applied AC signal.

[1] B. Kiraly et al., Nat. Nanotechn. 16, 414 (2021).
[2] B. Kiraly et al., Nat. Comm. 9, 3904 (2018).
[3] B. Kiraly et al., Phys. Rev. Research 4, 033047 (2022).

O 59.7 Wed 12:00 H6

**Spin-surface interactions of S=1/2 molecular magnets on superconductors** — •Susanne Baumann[1], Lukas Arnhold[1], Nicolaj Betz[1,2], Matteo Briganti[3], Andrea Sorrentino[4], Giulia Serrano[4], Federico Totti[3], Roberta Sessoli[3], 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, Stuttgart, Germany — [3]Department of Chemistry 'Ugo Schiff', University of Florence, Italy — [4]Department of Industrial Engineering, University of Florence, Italy

The interaction between magnetic molecules and superconducting surfaces critically depends on the electronic properties of the surface and the molecules' binding configuration, which determines the wave function overlap between molecule and surface. Using scanning tunneling microscopy (STM), we study the organometallic molecule (($\eta$8-cyclooctatetraene)($\eta$5-cyclopentadienyl)titanium) (CpTicot) on two different superconducting surfaces. On lead (Pb) nanoislands on Si(111), CpTicot exhibits multiple binding orientations with varying surface coupling strengths, that can be strong enough to generate Yu-Shiba-Rusinov bound states within the superconducting gap. Conversely, on vanadium (V(100)), the molecules adsorb in a single orientation with minimal coupling to the superconductor. Their spin states remain largely decoupled from the substrate, preserving their S=1/2 properties. These findings offer valuable insights into chemical design principles for molecular qubits where individual adressability and decoupling from superconducting substrates is desired.

O 59.8 Wed 12:15 H6

**Edge states in bottom-up designed spin chains on a superconducting Rashba surface alloy** — •Harim Jang, Khai That Ton, Lucas Schneider, Jens Wiebe, and Roland Wiesendanger — Department of Physics, University of Hamburg, Hamburg, Germany

The experimental quest for topological superconductors and emergent Majorana modes (MMs) at their edges have attracted significant interest recently in both directions of fundamental understanding of topology-driven quantum states and their potential applications in quantum computation leveraging the robustness by topological protection. A spin chain on a conventional superconductor in the presence of spin-orbit coupling is one of the promising platforms for realizing topologically non-trivial Yu-Shiba-Rusinov (YSR) bands, which can show signatures of MMs at the chain boundaries in the form of zero-energy states [1]. In this talk, we report on bottom-up designed Fe chains on the Rashba surface-alloy BiAg$_2$ grown on Ag(111)/Nb(110) and the detailed investigation of prominent states near the Fermi level at both chain ends, which are studied using scanning tunneling spectroscopy at sub-Kelvin temperatures. The atomically constructed Fe chains on the BiAg$_2$ alloy with proximity-induced superconductivity originating from the bulk Nb substrate show YSR bands with minigaps on the verge of our energy resolution inside the chain and edge states near the Fermi level at the chain's ends. The results are systematically compared to chains composed of other $3d$ transition metals, Mn and Co, on the same surface, revealing the absence of edge states for both cases. [1] S. Rachel and R. Wiesendanger, Phys. Rep. 1099, 1 (2025)

O 59.9 Wed 12:30 H6

**Second harmonic driving of paramagnetic resonance of molecular spin through non-linear transport phenomena** — •Stepan Kovarik[1], Richard Schlitz[1], Jose Reina-Gálvez[2,3], Aishwarya Vishwakarma[1], Dominic Ruckert[1], Nicolas Lorente[4,5], Christoph Wolf[2,3], Pietro Gambardella[1], and Sebastian Stepanow[1] — [1]ETH Zurich, Switzerland — [2]QNS, Seoul, Korea — [3]Ewha Woman University, Seoul, Korea — [4]CFM, Donostia-San Sebastian, Spain — [5]DIPC, Donostia-San Sebastian, Spain

The second harmonic excitation of electron paramagnetic resonance (EPR) originates from nonlinear processes. In this talk, I will demonstrate the presence of second and higher harmonic driving of a single spin in a pentacene molecule on 2ML MgO on Ag(001) when applying a radio-frequency electric field in an STM. Comparing our results to a theory considering EPR driven by a periodic modulation of the tunneling barrier [1] yields qualitative agreement, indicating the presence of higher harmonic driving. The key observation is that the barrier modulation can introduce nonlinearities to the electronic transport, leading to the excitation of magnetic resonance at the driving frequency [2] and at its multiples. Our work enhances the capabilities of EPR measurements in STM by introducing the frequency upconversion mechanism, showcasing the key role of electronic transport in driving the EPR. The presented findings apply also to other quantum transport systems, where the electrons are transported through discrete energy levels. References: [1]J. Reina-Gálvez et al., Phys. Rev. B 107, 235404 (2023)., [2]S. Kovarik et al., Science 384, 1368-1373 (2024).

O 59.10 Wed 12:45 H6

**A quantum simulator to study electronic structure of matter in the Hofstadter limit** — •Hermann Osterhage, Julian H. Strik, Kira Junghans, Niels P. E. van Mullekom, Anna M. H. Krieg, Emil Sierda, Danis Badrtdinov, Daniel Wegner, Mikhail I. Katsnelson, Malte Rösner, and Alexander A. Khajetoorians — Radboud University, Nijmegen, The Netherlands

The Hofstadter limit describes electronic structure in strong magnetic fields, where the magnetic length is on the order of the periodicity of the crystal. In this limit, the electronic structure shows self-similarity, namely fractal behavior. Experimentally, it is challenging to reach this limit for conventional crystals due to the high required field strengths. Therefore, one solution is to investigate structures with effectively larger periodicities. [1]. However, finding platforms that allow to study this limit with control over orbital and lattice symmetries is a current challenge.

Here, I will present a quantum simulator based on patterning Cs atoms on the surface of InSb(110) by scanning tunneling microscopy [2]. Cs atoms can be patterned into nanostructures that exhibit multi-orbital wavefunctions reminiscent of an artificial atom, and can be coupled to each other. We detail how the electronic spectrum evolves in magnetic field, and discuss the role of finite size effects and temperature, as well as link this to the expected spectra in the Hofstadter limit.

[1] R. Krishna Kumar et al., Science 357, 181 (2017).
[2] E. Sierda, et al, Science 380, 1048 (2023).

## O 60: Plasmonics and Nanooptics: Fabrication, Characterization and Applications I

Time: Wednesday 10:30–12:45 Location: H8

O 60.1 Wed 10:30 H8

**Infrared beam-shaping via geometric phase metasurfaces with the plasmonic phase-change material In$_3$SbTe$_2$** — •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$_3$SbTe$_2$ (IST) [1] 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.[2] [1] Heßler et al. *Nat. Com.* **12**, 924 (2021) [2] Conrads et al. *arXiv:2408.05044* (2024)

O 60.2 Wed 10:45 H8

**Investigation of lithiated carbon as active plasmonic material system** — •Valentin Maile, Mario Hentschel, and Harald Giessen — 4th Physics Institute, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Active plasmonic structures are integral to recent advancements in optical technologies due to their ability to confine and manipulate light on the nanoscale, enabling the miniaturization of optical devices. A pivotal aspect of future devices is the switchability and tunability of their optical resonances. However, only very few material systems can intrinsically switch the ability of the individual resonator to support plasmonic resonances via a metal-to-insulator transition.

Here, we introduce a novel concept based on lithium-intercalated carbon, a material system widely studied in battery research. The electrically driven, reversible lithium intercalation in the carbon lattice leads to an increase in charge carrier density and a corresponding shift in the optical material properties, visibly changing its color from black to golden. This unique optical modulation demonstrates its potential for integrating dynamic plasmonic functionalities.

In this work, lithiated forms of carbon and their change in optical reflectance are investigated as a switchable material system for plasmonics. Furthermore, we explored multiple fabrication techniques for nanostructuring the material, demonstrating that the nanostructures can be electrically switched while maintaining their structural integrity. This approach promises to expand the toolkit of active plasmonic structures for metasurfaces and nano-optics.

O 60.3 Wed 11:00 H8

**Hybrid resonant metasurfaces combining dielectric nanocup metasurfaces and plasmonic networks** — Jelena Wohlwend, Anna Hilti, Claudiadele Polinari, Ralph Spolenak, and •Henning Galinski — Laboratory for Nanometallurgy Department of Materials ETH Zurich, 8093 Zurich, Zurich Switzerland

State-of-the-art dielectric metasurfaces commonly consist of geometric primitives, such as cylinders or nanofins, and their integration into hybrid systems is fundamentally limited as confinement of light occurs only in their interior. In this talk, we report on a simple fabrication scheme that unlocks a new degree of freedom in the optical design space, as it enables the design of complex metasurfaces that break the out-of-plane symmetry [1]. We showcase the versatility of this approach on the specific example of nanocup metasurfaces made of amorphous silicon. We outline the extraordinary modal properties of these resonant sub-wavelength structures including confinement of light in air, lattice resonances and optical non-reciprocity. Creating complex hybrid metasurfaces, which combine such ordered silicon nanocups and disordered plasmonic networks [2, 3], we demonstrate that the generation of configurable structural colors can be tailored by the local near-field coupling between the ordered and disordered optical elements.

References: [1] Adv. Optical Mater. 2024, 12, 2401501. [2] Adv. Optical Mater. 2023, 11, 2300568. [3] Nano Letters 2022, 22 (2), 853-859

O 60.4 Wed 11:15 H8

**Optical programming of Hyperbolic Phonon Polariton Res-**

**onators with the plasmonic phase-change material $In_3SbTe_2$** — •Aaron Moos, Lina Jäckering, Lukas Conrads, Matthias Wuttig, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Germany

Tailoring light at the nano scale is mandatory for creating new nanophotonic devices and is achievable with polaritons. Hexagonal Boron Nitride (hBN), a 2d van der Waals material, hosts Hyperbolic Phonon Polaritons (HPPs) featuring high volume-confinement and low losses [1]. Restricting HPPs to resonators enables ultra-confined resonances, but their fabrication requires cumbersome etching processes [2]. Instead, resonators can be fabricated via optical programming of a phase-change material like $In_3SbTe_2$ (IST) with a metallic and a dielectric state in the infrared enabling rapid fabrication and reconfigurability. IST resonators combined with surface polaritons on bulk SiC were exploited before [3]. Here, we show optical programming of circular IST resonators below 2d hBN and investigate the HPP mode structures with scattering-type scanning near-field optical microscopy (s-SNOM). Influences of hBN thickness and resonator-size on resonances are studied. Furthermore, we show focussing of free propagating HPPs launched by a crystalline IST structure with tuneable focal length by reconfiguring. Our results enable rapid prototyping of confined polariton resonators for infrared nanophotonics. [1] Dai et al., *Science* **343**, 1125-1129 (2014), [2] Sheinfux et al., *Nat. Mat.* **23**, 499-505 (2024), [3] Conrads et al., *Nat. Com.* **15**, 3472 (2024)

O 60.5 Wed 11:30 H8

**Optical Response of High-refractive Index Nanodisk Arrays with Hyperuniform Disorder** — •Davy Tesch, Koundinya Upadhyayula, Bodo Fuhrmann, Alexander Sprafke, and Ralf Wehrspohn — Martin Luther University Halle-Wittenberg, 06120 Halle, Germany

Light-scattering metasurfaces with tailored disorder, in particular hyperuniform disorder (HUD), have recently attracted interest in the photonics community. HUD promises several properties that were previously associated only with either periodic or random structures. The combination of the strong diffraction of periodic structures and the broadband spectral response of disordered structures holds promise for tailored light scattering.

In this work, we use a scalable fabrication process to experimentally fabricate HUD nanodisk arrays using hydrogenated amorphous silicon (a-Si:H) optimised for low absorption as the nanodisk material. Optical measurements of such fabricated samples show a strong dependence of the scattering response on the form factor of the individual scatterers and their HUD arrangement, given by the structure factor. By tuning these quantities, we were able to tailor the scattering response. One of the most striking results is the ability of the fabricated samples to suppress scattering at small angles (below 45°) due to the HUD arrangement and to enhance scattering at large angles (up to 80°) due to the dominance of electric dipoles in single a-Si:H scatterers.

We have also studied a more complex system: nanodimers consisting of two stacked nanodisks, separated by a spacer layer.

O 60.6 Wed 11:45 H8

**Edge-state imaging of high-precision plasmonic SSH chains** — Benedikt Schurr[1], Luisa Brenneis[2], Philipp Kessler[2], Jin Qin[1], Victor Lisinetskii[2], •Matthias Hensen[2], Ronny Thomale[3], Tobias Brixner[2], and Bert Hecht[1] — [1]NanoOptics & Biophotonics Group, Experimental Physics 5, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Institute for Theoretical Physics and Astrophysics, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Topological nanophotonics offers the possibility to precisely control nanoscale light–matter interaction via states that are topologically protected from disorder and impurities. A prominent example are Su–Schrieffer–Heeger (SSH) chains, in which the staggered nearest-neighbor coupling strength leads to topologically protected and localized edge states. Here, we present plasmonic SSH chains of nanoslot dipole antennas fabricated by helium ion-beam milling in a single-crystal Au micro-platelet. The chains are characterized by individual antenna distances down to 12 nm, strong coupling amplitudes, and negligible next-nearest-neighbor coupling. Furthermore, the near-field distribution of plasmonic eigenmodes is consistent with the amplitude distribution of the eigenfunctions of a quantum mechanical SSH model. We prove the existence of topological edge states experimentally by imaging corresponding mode patterns with aberration-corrected photoemission electron microscopy (PEEM) under wide-field excitation.

O 60.7 Wed 12:00 H8

**Analytical study of Mie void resonances** — Timothy J. Davis[1,2], •Julian Schwab[1], Harald Giessen[1], and Mario Hentschel[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

The preferential light scattering at particular wavelengths by mall particles is a well know phenomenon since the introduction of an analytical theory by Gustav Mie in 1908. Over the decades, this theory has helped in understanding, designing, and optimizing a multitude of plasmonic and dielectric nanophotonic systems. Just recently it was shown that Mie scattering can also be observed from voids in high-index dielectric media, such as silicon or gallium arsenide. This phenomenon is particularly counterintuitive as the void sizes are on the order of the resonant wavelength, rendering full-wave simulations and thus a deeper understanding challenging. Here, we present a new analytical model to study and understand the resonance properties of Mie voids. In particular, we derive analytical expressions of the electric field distribution based on solutions of Maxwell's equations for cylindrical holes in the substrate. These solutions are used in a simple three-layer model of the void that gives predictions of the void resonances, the observed spectra, as well as the microscopic appearance. Our model will aid in the future design of Mie-void based systems and applications, such as nanophotonic sensors, metasurfaces, and nanoscale detection.

O 60.8 Wed 12:15 H8

**In-situ Plasmonic Sensing of Surfactant Structures** — •Esmée Berger[1], Narjes Khosravian[1], Ferry Nugroho[2], Joakim Löfgren[3], Christoph Langhammer[1], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Department of Physics, Universitas Indonesia, Depok, Indonesia — [3]Department of Applied Physics, Aalto University, Espoo, Finland

Surfactants play an important role in many areas of chemistry and have immense technological relevance. Their functionality is dictated by their frequently complex phase diagrams, which are very difficult to probe, especially *in situ*. Here, by combining experiment and multiscale modeling, we demonstrate that the structure and dynamics of surfactant layers can be very efficiently probed using plasmonic sensing. Considering a prototypical surfactant-surface system (CTAB on silica), we show that the plasmonic response not only reveals changes in the structure of the surfactant layer as the CTAB concentration varies but also provides access to the kinetics of the phase transition. The approach demonstrated in the present work is minimally intrusive, efficient, and widely applicable. It thus constitutes a very powerful tool for exploring surfactant-surface structures, representing a large step forward in understanding these systems of enormous scientific and technological importance.

O 60.9 Wed 12:30 H8

**Optical Sieve for Nanoplastic Detection** — •Dominik Ludescher[1], Lukas Wesemann[2], Julian Schwab[1], Julian Karst[1], Shaban B. Sulejman[2], Monika Ubl[1], Ann Roberts[2], Harald Giessen[1], and Mario Hentschel[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]ARC Center of Excellence for Transformative Meta-Optical Systems (TMOS), The University of Melbourne, Australia

Micro- and nanoplastics contaminate marine ecosystems and endanger aquatic life, even in remote locations. These minute synthetic fragments, persisting for hundreds of years, infiltrate the food chain, posing potential health risks due to toxic chemicals. Besides improving the quality of plastic disposal and reducing plastic production, determining the existence of micro- and nanoplastics in aqueous environments like water or blood is essential for biological studies. We present an optical sieve for nanoplastic detection based on the recently discovered Mie void resonances. Our devices are able to detect, size, and count nanoplastic particles by observing apparent color changes of the emitted light in the presence of a sphere in the void. The proposed method profits from its simplicity and only requires a conventional microscope setup with CMOS RGB imaging sensor.

# O 61: 2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)

Time: Wednesday 10:30–12:45 Location: H11

O 61.1 Wed 10:30 H11

**The Bell-Shaped Component in Diffraction from 2D Materials** — •Birk Finke[1], Christian Brand[1], Karim Omambac[1,2], Pascal Dreher[1], Hannah Kohler[1], Frank-J. Meyer zu Heringdorf[1,3,4], and Michael Horn-von Hoegen[1,3] — [1]Universität Duisburg-Essen — [2]Polytechnique Montréal Canada — [3]Center for Nanointegration Duisburg-Essen — [4]Interdisciplinary Center for Analytics on the Nanoscale

In 2D materials, the formation of moiré superlattices with graphene or hBN on crystalline surfaces alters electronic, vibrational, and chemical properties. Here we analysed an unusual broad diffraction background observed in low energy electron diffraction from 2D material systems, which is called the bell-shaped component (BSC). Employing SPA-LEED, LEEM, and $\mu$-LEED we propose the origin to be the inelastic scattering of the low energy electrons at the vertically polarized ZA-phonons of the weakly bound graphene and hBN layers on Ir(111) and SiC(0001). For these systems the ZA-phonon branch exhibits a parabolic dispersion with a finite phonon frequency of a few meV at the $\Gamma$ point. This results in a high phonon density at low energy, but high momentum causing the strong intensity of the BSC in diffraction. In the framework of kinematic scattering theory, we performed simulations of the inelastic diffuse scattering which quantitively confirm our proposal.

O 61.2 Wed 10:45 H11

**Combining DFT and ML to Explore the Electronic Properties of Nano-porous Graphene** — •Bernhard Kretz and Ivor Lončarić — Institut Ruder Bošković, Zagreb, Croatia

Nano-porous graphene (NPG) holds great potential in electronics due to its tunable electronic properties. However, establishing a comprehensive understanding of how structural parameters influence these properties remains a challenge. This work employs density functional theory (DFT) calculations combined with machine learning (ML) to systematically investigate both static and dynamic electronic properties across a set of 460 NPG structures derived from four distinct templates.

Our DFT results reveal correlations between structural features and band gaps within subsets of our NPG structures. Notably, we identify certain NPG configurations exhibiting band gap behavior analogous to armchair graphene nano-ribbons. To predict the dynamic response of our NPG structures, we train two distinct ML networks: one for predicting forces and total energies, and another one for predicting band gaps. Using the former allows us to perform temperature-dependent molecular dynamics simulations for all 460 NPG structures, while the latter enables us to predict band gap evolution under varying operating temperatures, a crucial factor for semiconductor device performance. Our findings identify several NPG structures exhibiting band gaps suitable for semiconductor applications while demonstrating sufficient thermal stability to function effectively at typical operating temperatures.

**Invited Talk** O 61.3 Wed 11:00 H11

**Polaritons in two-dimensional materials and hybrids probed by electron beams** — •Nahid Talebi — Institute for Experimental and Applied Physics, Kiel University, Leibnizstr. 19, 24118 Kiel

Polaritonic quasiparticles in two-dimensional (2D) materials have garnered significant attention in recent years, emerging as a promising platform for studying novel photon- and phonon-mediated correlations between various material excitations. In this work, we employ electron beams to investigate exciton and plasmon polaritons in diverse 2D materials, including transition-metal dichalcogenides, perovskites, hexagonal boron nitride, borophene, and hybrid systems. By comparing cathodoluminescence and photoluminescence spectroscopy, we uncover differences in the selection rules governing the excitation of quasiparticles by coherent light versus electron beams. Furthermore, leveraging a recently developed method that utilizes electron-driven photon sources inside an electron microscope for Ramsey-type spectroscopy, we examine the coherence of cathodoluminescence emitted by exciton polaritons (Nature Physics 19, 869 (2023)) and defects in hexagonal boron nitride (arXiv:2404.09879). These results provide new insights into the temporal coherence of the radiation from 2D materials excited by coherent and incoherent excitations.

O 61.4 Wed 11:30 H11

**Electron-phonon interaction in polar two-dimensional materials** — •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 recently developed a generally applicable ab-initio implementation on top of density functional theory that 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 using a basis set of localized Gaussian orbitals. Our implementation circumvents the limiting problems of previous implementations and allows to evaluate Debye-Waller contributions beyond the rigid-ion approximation, which are usually neglected [1].

Incorporating effects from macroscopic electric fields into our implementation allows us to extend our calculations to the class of polar materials. In this presentation we discuss our results 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 61.5 Wed 11:45 H11

**Structural modulations of unidirectional charge density waves in rare earth tellurides** — •Eunseo Kim[1], Sanghun Lee[1], Junho Bang[1], Hyungryul Yang[1], Jongho Park[2], Changyoung Kim[2], Dirk Wulferding[2], Doohee Cho[1], Makoto Hashimito[3], Donghui Lu[3], and Sunghun Kim[4] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Republic of Korea — [3]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [4]Department of Physics, Ajou University, Suwon 16499, Korea

Charge density waves (CDWs) in rare earth tellurides ($RTe_3$) provide a unique platform for exploring the interplay between lattice deformations and electronic order. Using scanning tunneling microscopy and spectroscopy (STM/S), we investigate unique surface features in two different materials, $GdTe_3$ and $DyTe_3$, that influence the CDW behavior. In $GdTe_3$, twin domain boundaries provide a static platform for observing the spatial "melting" of unidirectional CDWs and the emergence of bidirectional CDWs. Our spatial lock-in analysis demonstrates the attenuation of CDW order parameters and the proliferation of topological defects at these boundaries, correlating with enhanced local density of states near the Fermi level. In $DyTe_3$, nanowrinkles act as topological interfaces, hosting phase-winding CDWs and confining one-dimensional metallic states. These findings emphasize the role of local structural distortions in shaping CDW phenomena, offering insights into manipulating quantum states via lattice engineering.

O 61.6 Wed 12:00 H11

**Ultrafast Charge Separation on the Nanoscale Induced by a Uniform Field** — •Jan-Philip Joost and Michael Bonitz — Kiel University, Institute for Theoretical Physics and Astrophysics, 24098 Kiel, Germany

When illuminated by white light, atoms, molecules, and materials absorb only certain characteristic energy contributions based on their absorption properties. Here, we show that this effect can be translated from energy to space: a spatially uniform laser pulse can create strongly localized carrier excitations and spatial charge separation on the sub-nanometer scale within a few femtoseconds, possibly opening new avenues for nanoelectronics. A promising candidate are small graphene heterostructures, which exhibit a pronounced space dependence of the DOS with strongly localized topologically protected states [1]. Direct evidence for this effect is presented by performing extensive NEGF simulations for these systems that take into account strong coupling and dynamical screening [2]. Further, we demonstrate multiple ways to excite targeted areas of the nanostructures, such as a proper choice of the laser energy, polarization, or carrier-envelope phase. Moreover, we find that the observed effects greatly benefit from surface screening, while in free-standing systems the targeted charge excitation is restricted by strongly bound excitons. The findings are expected to be applicable for a broad class of nanoscale monolayer clusters of graphene or TMDCs.

[1] J.-P. Joost et al., Nano Lett. **19**, 9045 (2019)
[2] J.-P. Joost et al., Phys. Rev. B **105**, 165155 (2022)

O 61.7 Wed 12:15 H11

**Two-dimensional breathing Kagome lattice of antimony atoms on a SiC substrate** — •Bing Liu[1], Kyungchan Lee[1], Jonas Erhardt[1], Manish Verma[1], Stefan Enyner[1], Cedric Schmitt[1], Philipp Kessler[1], Lukas Gehrig[1], Chris Jozwiak[2], Aaron Bostwick[2], Martin Kamp[1], Eli Rotenberg[2], Jörg Schäfer[1], Simon Moser[1], Giorgio Sangiovanni[1], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

The Kagome lattice, characterized by flat electronic bands, which represents a class of candidate materials for charge order, time-reversal symmetry-breaking and exotic superconductivity. In this work, we report the successful synthesis of a breathing Kagome lattice of Sb on SiC surface. Band mapping reveals a significant gap opening at the K point near the Fermi level, driven by different hopping parameters within the breathing Kagome lattice. Scanning tunneling microscopy measurements of this phase confirm a well-ordered 2x2 lattice reconstruction, consistent with the breathing Kagome unit cell. Furthermore, DFT calculations elucidate the role of the Sb p-orbitals. Specifically, near the Fermi level the physics is dominated by px and py orbitals, which are sensitive to hopping and possibly electron correlation, giving rise to an energy gap, and by their splitting reflect the breathing Kagome lattice situation. Our findings demonstrate a pathway for constructing two-dimensional Kagome lattices on semiconductor surfaces, and are encouraging further research into their spin and electronic properties.

O 61.8 Wed 12:30 H11

**Ultrafast lattice dynamics of monolayer $ReS_2$** — •Victoria C. A. Taylor[1], Yoav W. Windsor[1,2], Samuel Lai[3], Hyein Jung[1,2], 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

Within the transition metal dichalcogenide (TMDC) material family, TMDCs containing rhenium stand out due to their low crystal symmetry. Instead of the common hexagonal structure, $ReS_2$ exhibits in-plane 1D chains of rhenium ions due to a Peierls-like distortion. This highly anisotropic crystal structure results in a range of material properties, such as anisotropic effective carrier masses, polarization dependent optical absorption, and extremely weak interlayer coupling.

We present femtosecond electron diffraction (FED) measurements of monolayer $ReS_2$. FED is a direct probe of photoexcited lattice dynamics, providing quantitative information on coherent and incoherent atomic vibrations on femtosecond timescales. In $ReS_2$ monolayers we observe a strong and complex lattice response to photoexcitation. In particular, we observe a rapid (<1 ps) collective response, indicative of a concerted change in ionic positions within the unit cell. We measure the fluence dependence of this response and investigate the effect of the pronounced polarization dependence of the optical excitation, which results from the material's in-plane anisotropy.

## O 62: Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation III

This focus session aims to discuss recent advances in the on-surface synthesis, manipulation, characterization, and understanding of complex molecular architectures on surfaces. The interest in surface-confined molecular nanostructures emerges from their prospective applications in nanoscale (opto-) electronics, spintronics, solar cells, energy storage devices, and other fields. The bottom-up fabrication of surface-supported nanostructures can be based on molecular self-assembly utilizing non-covalent intermolecular interactions, covalent on-surface synthesis, or the direct manipulation of molecules. Molecular self-assembly usually leads to highly ordered nanostructures, controlled by non-covalent interactions, adsorbate-substrate interactions, as well as thermodynamic and kinetic factors. On-surface synthesis by covalent coupling of reactive precursors adsorbed on metallic, semiconducting, or even insulating surfaces has emerged as a powerful method that has opened new possibilities in exploring new routes towards the synthesis of complex low-dimensional nanostructures with unprecedented material properties, often via novel chemical reactions not available in conventional organic chemistry. Finally, the direct manipulation of molecules with the tip of a scanning probe microscope allows for unprecedented chemical transformations or structural modifications, as envisioned by the pioneers of nanotechnology. This focus session is intended to provide a platform for addressing current trends in these closely linked fields from various perspectives in experiment and theory.

Organized by
Sabine Wenzel (University of Marburg) and Christian Wagner (Forschungszentrum Jülich)

Time: Wednesday 10:30–13:00 Location: H24

O 62.1 Wed 10:30 H24

**Selective On-Surface Synthesis of Isokekulene Facilitated by Strong Molecule-Substrate Interaction** — Qitang Fan[1], Alexander Reichmann[2], Zilin Ruan[1], Faming Kang[1], Tim Naumann[1], Simon Werner[1], Olaf Kleykamp[1], Jose Martinez[3], Felix Lüpke[3], François C. Bocquet[3], Christian Kumpf[3], Serguei Soubatch[3], Jörg Sundermeyer[1], Peter Puschnig[2], F. Stefan Tautz[3], J. Michael Gottfried[1], and •Sabine Wenzel[1,3] — [1]Fachbereich Chemie, Philipps-Universität Marburg — [2]Institute of Physics, University of Graz — [3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich

The role of different facets of metal nanoparticles in steering reaction pathways is crucial for the design of heterogeneous catalysts with superior selectivity. Transition-metal-catalyzed C-H bond activation is widely used for the synthesis of different chemicals. Here, we report orthogonal selectivity in intramolecular cyclodehydrogenation of a nonplanar cyclic precursor steered by different facets of a copper single crystal. On Cu(110), the previously unknown cycloarene isokekulene is formed with a high selectivity of 92 %, while reaction on Cu(111) is known to result in kekulene (> 99 %). Combining scanning tunneling microscopy with CO-functionalized tips and density functional theory, we identify two adsorption geometries of the precursor which react to the respective products. The isokekulene molecule appears in two nonplanar adsorption configurations and shows a strong molecule-substrate interaction including charge transfer, which accounts for the more favorable energetics of isokekulene on Cu(110).

O 62.2 Wed 10:45 H24

**On-surface synthesis and characterization of long azaacenes** — •Zilin Ruan[1], Liping Ye[2], Jakob Schramm[3], Tim Naumann[1], Faming Kang[1], Ralf Tonner-Zech[3], Michael Mastalerz[2], and

J. Michael Gottfried[1] — [1]Department of Chemistry, Philipps-Universität Marburg, 35037 Marburg, Germany — [2]2Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, 69120 Heidelberg, Germany — [3]Wilhelm Ostwald Institute of Physical and Theoretical Chemistry, Universität Leipzig, 04103 Leipzig, Germany

Introducing electronegative nitrogen into the backbone of acenes yields azaacenes, enabling fine-tuning of the energy alignment of frontier orbitals while enhancing resistance to oxidation, photodegradation, and dimerization. Here, we demonstrate the on-surface synthesis of tetraazanonacene and hexaazatridecacene, the latter being the longest azaacene known to date and here reported for the first time via atom-manipulation-induced dissociation of a trietheno-bridged precursor on a Au(111) surface in UHV. The geometric and electronic structures of the generated azaacenes were investigated by combined scanning tunneling microscopy/spectroscopy and non-contact atomic force microscopy. For tetraazanonacene, we observed an increase of the frontier orbital gap compared to pristine nonacene, attributed to a more pronounced downshift of occupied states. Meanwhile, hexaazanonacene exhibited an open-shell singlet ground state with a singlet-triplet gap of 110 meV, slightly smaller than that observed for long acenes.

O 62.3 Wed 11:00 H24

**On-surface synthesis and characterization of polyynic carbon chains** — •Wenze Gao[1,2], Wei Zheng[1], Luye Sun[1], Faming Kang[1], Zheng Zhou[1], and Wei Xu[1] — [1]Interdisciplinary Materials Research Center, School of Materials Science and Engineering, Tongji University, Shanghai, China — [2]Empa-Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

Carbyne, an elusive sp-hybridized linear carbon allotrope, has fascinated chemists and physicists for decades. Due to its high chemical reactivity and extreme instability, carbyne was much less explored in contrast to the sp2-hybridized carbon allotropes such as graphene. Herein, we report the on-surface synthesis of polyynic carbon chains by demetallization of organometallic polyynes on the Au(111) surface; the longest one observed consists of 60 alkyne units (120 carbon atoms). The polyynic structure of carbon chains with alternating triple and single bonds was unambiguously revealed by bond-resolved atomic force microscopy. Moreover, an atomically precise polyyne, C14, was successfully produced via tip-induced dehalogenation and ring-opening of the decachloroanthracene molecule (C14Cl10) on a bilayer NaCl/Au(111) surface at 4.7 K, and a band gap of 5.8 eV was measured by scanning tunnelling spectroscopy, in a good agreement with the theoretical HOMO-LUMO gap (5.48 eV).

O 62.4 Wed 11:15 H24

**The odd-number cyclo[13]carbon and its dimer, cyclo[26]carbon** — •Florian Albrecht[1], Igor Rončević[2], Yueze Gao[2], Fabian Paschke[1], Alberto Baiardi[3], Ivano Tavernelli[3], Shantanu Mishra[1], Harry L. Anderson[2] und Leo Gross[1] — [1]IBM Research Europe - Zurich — [2]Department of Chemistry, Oxford Univeristy — [3]IBM Quantum, IBM Research Europe - Zurich

Using CO-functionalized tips, we generate the odd-numbered cyclocarbon molecule cyclo[13]carbon (C13) on an ulatra-thin insulating film by applying voltage pulses to a stable precursor molecule. The geometric and electronic properties of C13 were characterized experimentally as well as theoretically, determining the electronic ground state to be an open-shell triplet. In addition to the C13 monomer, we also generated its dimer, cyclo[26]carbon, from two precursor molecules [1].

[1] Albrecht et al., Science 384, 677 (2024)

**Invited Talk** O 62.5 Wed 11:30 H24

**On-Surface Synthesis with Hydrogen Atoms** — •Szymon Godlewski — Jagiellonian University, Krakow, Poland

In recent years the on-surface manipulation and chemical reactions created a playground for atomically precise synthesis and development of new atomic and molecular nanostructures. However, the abilities to produce desired systems are limited, among others, by relying on the catalytic role of the substrate in initiating selected reactions. Therefore striving for the generation of desired systems forces the search of new reaction pathways and catalytic transformations.

In this talk I will demonstrate our approach based on the application of hydrogen atoms in the on-surface experiments. First, I will discuss the synthesis of the acene series based on the application of *extra* hydrogen atoms. The application of atomic hydrogen in on-surface transformations will be exemplified by organometallic hybrids and graphene nanoribbons.

While the surface assisted synthesis approach has proven its effectiveness in the precise formation of new organic compounds on metallic surfaces one of the most challenging limitations arises from the dependence on the catalytic activity of the substrate. This makes the direct transfer to the non-metallic surfaces extremely challenging. In this talk I will present our pathway for the synthesis of new molecular compounds on non-metallic surfaces with prospects for circumventing the need to exploit the catalytic role of metallic substrates.

This work was supported by the National Science Center, Poland (2019/35/B/ST5/02666)

O 62.6 Wed 12:00 H24

**On-Surface Synthesis of Hydrogen-Substituted $\gamma$-Graphdiyne with High Efficiency** — •Faming Kang[1,3], Wei Zheng[1], Luye Sun[1], Wenze Gao[1], Lina Shang[1], Lifeng Chi[2], and Wei Xu[1] — [1]Interdisciplinary Materials Research Center, School of Materials Science and Engineering, Tongji University, 201804 Shanghai, China — [2]Institute of Functional Nano & Soft Materials (FUNSOM), Jiangsu Key Laboratory for Carbon-Based Functional Materials and Devices, Joint International Research Laboratory of Carbon-Based Functional Materials and Devices, Soochow University, 215123 Suzhou, China — [3]Department of Chemistry, University of Marburg, 35032 Marburg, Germany

Graphyne-family structures, a group of hybrid carbon allotropes with sp- and sp2-hybridized carbon atoms, are expected to have unique features, including a natural direct bandgap, unlike graphene. Here, we developed and synthesized precursors with one and three tribromoethenyl groups. In mild conditions, metal-free dimer and network (HsGDY) products were synthesized in big scale and good quality. The geometric structure of synthesized dimer and network products was accurately characterized by scanning tunneling microscopy and non-contact atomic force microscopy. The electronic structures of produced hydrogen-substituted graphdiyne were studied using DFT calculations. Our research may motivate theoretical and experimental efforts to create more sensitive two-dimensional carbon nanostructures with sp-hybridized carbon atoms.

O 62.7 Wed 12:15 H24

**Tip-induced nitrene generation** — •Leonard-Alexander Lieske[1], Aaron Oechsle[1], Ilias Gazizullin[2], Matthias Krinninger[3], Igor Rončević[4], Florian Albrecht[1], Leonhard Grill[2], Friedrich Esch[3], and Leo Gross[1] — [1]IBM Research Europe - Zurich, Rueschlikon, Switzerland — [2]Physical Chemistry Department, University of Graz, Graz, Austria — [3]Chair of Physical Chemistry and Catalysis Research Center, Department of Chemistry, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [4]Department of Chemistry, University of Manchester, Manchester, United Kingdom

We have successfully generated mono-, di- and trinitreno-*s*-heptazine by tip-induced chemistry from the precursor 2,5,8-triazido-*s*-heptazine[1,2] on bilayer NaCl and on bare Au(111). The precursor's azide groups are cleaved off sequentially in a controlled manner, demonstrating the generation of single molecules with one, two and three nitrene moieties, which are highly reactive.[3] We characterized the mono-, di- and trinitrene species by high-resolution atomic force microscopy with CO functionalized tips[4] and by scanning tunneling microscopy. Broken-symmetry density functional theory and multireference complete active space calculations of inter- and intra-nitrene exchange couplings $J$ and $J*$ suggest a high-spin ($S = 3$) ground state for trinitreno-*s*-heptazine. [1] D. Miller et al., *J. Am. Chem. Soc.*, 126, 5372 (2004). [2] M. Krinninger et al., *Chem. Mater.*, 35, 6762 (2023). [3] M. Janssen et al., *Science*, 385, 318 (2024). [4] L. Gross et al., *Science*, 325, 1110 (2009).

O 62.8 Wed 12:30 H24

**On-Surface Synthesis and Reactivity of Biphenylene Network on Au(788)** — •Ye Liu, Yingling Zhang, Zilin Ruan, Tim Naumann, Faming Kang, Ulrich Koert, and J. Michael Gottfried — Department of Chemistry, University of Marburg, 35032 Marburg, Germany

The recently synthesized biphenylene network (BPN), a new sp2-hybridized carbon allotrope comprising four-, six-, and eight-membered rings, significantly differs from graphene in its electronic and chemical properties. Theoretical studies predict that BPN features a multiradical ground state, with its open-shell character predominantly localized at the four-membered rings. However, experimental confirmation of these predictions has been hindered by the limited quality of the material currently available. To address this challenge, we employed Au(788), a surface characterized by narrow terraces, and designed an extended molecular precursor to promote the formation of the desired structure. For comparison, we also investigated interpolymer dehydrofluorination (HF-zipping) reactions of the precursor on Au(111). Scanning probe microscopy (SPM) analysis revealed that pure BPN fused chains formed on Au(788) exhibit superior structural quality compared to those synthesized on Au(111). These findings provide a solid experimental foundation for probing the theoretically predicted properties of BPN, opening avenues for the further exploration of its distinctive electronic and chemical behavior.

O 62.9 Wed 12:45 H24

**Incorporating Nonhexagonal Polygons into Carbon-Based Nanostructures via On-Surface Synthesis** — •Dong Han[1], Jakob Schramm[2], Zilin Ruan[1], Tim Naumann[1], Konstantin Y. Amsharov[3], Ralf Tonner-Zech[2], and J. Michael Gottfried[1] — [1]Department of Chemistry, Philipps-Universität Marburg, Marburg, Germany — [2]Faculty of Chemistry and Mineralogy, Wilhelm Ostwald Institute for Physical and Theoretical Chemistry, Universität Leipzig, Leipzig, Germany — [3]Institute of Chemistry, Organic Chemistry, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

The incorporation of nonhexagonal rings offers a powerful strategy for designing novel carbon-based nanostructures with unique physicochemical properties. Herein, we report the on-surface synthesis of: (1) Quasi-planar, furan-containing cycloparaphenylenes (CPPs): Synthesized via Ullmann coupling and cyclodehydrogenation on Au(111), these CPPs show a decreasing energy gap with increasing size. Orbital confinement at edges and pores is observed, which is associated with the slower wave function decay above the CPP plane. (2) Carbon nanoribbons (CNRs) embedded with nonbenzenoid rings: Zigzag nanoribbons bearing 5-6-7 membered rings and linear nanoribbons containing 4-5-6-8 carbon polygons are formed through the lateral fusion of polymer chains on Au(111). Low-temperature scanning tunneling microscopy/spectroscopy (STM/STS) reveals their geometric and electronic properties, and X-ray photoelectron spectroscopy (XPS) unravels the reaction process.

## O 63: Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules II

Time: Wednesday 10:30–12:30 Location: H25

O 63.1 Wed 10:30 H25

**Unravelling the Photocatalysis of Alcohol on Rutile(110)** — •Philip Petzoldt, Lucia Mengel, Anna Lemperle, Moritz Eder, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Heterogeneous photocatalysis is a promising tool for the environmentally benign production of chemical fuels such as hydrogen. However, the structural complexity of state-of-the-art materials makes mechanistic investigations and, in consequence, the targeted design of new catalysts extremely challenging. We employ surface science methods to explore fundamental mechanisms in photocatalysis. In this contribution, we focus on the photocatalytic hydrogen evolution from alcohols over rutile(110) loaded with Pt cluster co-catalysts. Our experimental evidence reveals a new reaction mechanism, which substantially differs from the generally assumed model of independent redox reactions. By changing active sites for both the alcohol oxidation and the hydrogen evolution reaction, we further show that the overall photoactivity strongly depends on the equilibrium of a reaction network of several elementary photo- and thermal reaction steps. Our results provide new mechanistic insights into the photocatalytic hydrogen evolution from Pt loaded titania and illustrate the importance of a comprehensive understanding of the photocatalysts (surface) chemistry.

O 63.2 Wed 10:45 H25

**Characterization of rhodium single atoms as dicarbonyls on $TiO_2$(110)** — •Moritz Eder, Faith Lewis, Panukorn Sombut, Johanna Hütner, David Rath, Jan Balajka, Jiri Pavelec, and Gareth Parkinson — Institute of Applied Physics, TU Wien, Austria

Single-atom catalysts (SACs) have garnered significant attention in recent years due to their potential to minimize noble metal usage by isolating active atoms on metal (oxide) surfaces. However, stabilizing these single atoms remains a major challenge. Ligands, such as carbon monoxide, can stabilize single atoms by transforming them into surface-bound metal complexes, closely resembling the well-defined species in homogeneous catalysis. In this contribution, we present a comprehensive characterization of a ligand-stabilized single atom: a rhodium gem-dicarbonyl ($Rh(CO)_2$) bound to rutile $TiO_2$(110). Using XPS, TPD, scanning probe, and a newly developed IRRAS apparatus, we provide a detailed analysis of these sites. Our findings are contextualized through comparisons with theoretical models and insights from powder catalyst studies in the literature. This work demonstrates that multi-technique approaches are essential for the accurate characterization of single-atom catalysts, offering a deeper understanding of their structure and stability.

O 63.3 Wed 11:00 H25

**Desorption of water from microcline (001)** — Tobias Dickbreder[1,2], Florian Schneider[1], Lea Klausfering[1], Kim Noelle Dreier[1], Franziska Sabath[1,3], Adam S. Foster[4], Ralf Bechstein[1], and •Angelika Kühnle[1] — [1]Bielefeld University, 33615 Bielefeld, Germany — [2]University of Vienna, 1090 Vienna, Austria — [3]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [4]Aalto University, Finland and Kanazawa University, Kanazawa 920-1192, Japan

Feldspar minerals are highly abundant in the Earth's crust. They play a significant role in a plethora of geochemical processes, including, e.g., weathering and ice nucleation. For many of these processes, the interaction of water with the feldspar surface is decisive. However, little is known about binding and desorption of the first water layer on feldspar. Here, we present temperature-programmed desorption (TPD) experiments of water desorbing from the thermodynamically most stable cleavage plane of potassium-rich feldspar, microcline (001). From the interplay of these experimental data with density-functional theory (DFT) results we shed light onto the binding of the first water layer. Our work confirms previous theory results from literature and provides molecular-scale insights into the binding of water onto microcline (001).

O 63.4 Wed 11:15 H25

**Cleaved feldspar surfaces under dry and humid conditions: an AFM study** — •Luca Lezuo[1], Sandra Boigner[1], Rainer Abart[2], Michael Schmid[1], Ulrike Diebold[1], and Giada Franceschi[1] — [1]Inst. of Applied Physics, TU Wien, 1040 Wien, Austria — [2]Dep. of Lithospheric Research, Universität Wien, 1090 Wien, Austria

The Earth's surface is largely shaped by the interaction between water and the minerals of its crust. Feldspars, the most common aluminosilicates, are made of a framework of corner-sharing silica and alumina tetrahedra, enclosing cations such as potassium ($K^+$), sodium ($Na^+$), and calcium ($Ca^{2+}$). The chemical reactions at the feldspar-water interface contribute to geological processes such as erosion and weathering [1], clay formation [2], and ice nucleation [3], with implications for geology, agriculture, atmospheric chemistry, and climate science.

We exposed cleaved surfaces of different feldspars to air and Ar with defined humidity and examined the evolution of their mesoscale morphology with atomic force microscopy (AFM). Overlayers with distinct patterns develop over time. They remain stable after rinsing the surface with ultrapure water, suggesting a permanent alteration of the surface morphology. We attribute the distinct patterns to local chemistry differences and different cation leaching rates [1].

[1] Brantley and White, Chem. Weath. Rates of Sil. Min. (2018)
[2] Bleam., Clay Min. and Chem., 87-146 (2017)
[3] Atkinson, et al., Nature 498, 355-358 (2013)

O 63.5 Wed 11:30 H25

**Tracking the redox cycle of $CeO_2$ by Infrared spectroscopy via a titration of the defect states by $O_2$ adsorption.** — •Lachlan Caulfield, Eric Sauter, Hicham Idriss, and Christof Wöll — Karlsruhe Institute of Technology

$CeO_2$ is probably the most stable reducible metal oxide known. It is the main component of automobile three-way catalysts and is the chief prototype for the thermochemical water splitting to $H_2$ and $O_2$ reaction as well as for $CO_2$ thermal reduction to CO. This is largely due to the relative stability of the $Ce4f_1$ electron formed upon the removal of surface oxygen atoms during the reduction process. While these are commonly studied by photoelectron spectroscopy (XPS Ce3d or UPS Ce4f), less attention in general has been given to the $Ce^{3+}$ (2F5/2 to 2F7/2) spin orbit transition of this process that appears in infrared spectroscopy at ca. 2150 $cm^{-1}$. In this work we have monitored the formation of these transition on reduced polycrystalline $CeO_2$ exposed to molecular $O_2$ as a function of temperature using the DRIFT technique. Results have shown that there is a linear relationship between the disappearance of the observed electronic transition at ca. 2130-2160 $cm^{-1}$ and the IR signal of the superoxo ($O^{2-}$). species upon exposure of the reduced surface to different partial pressures of $O_2$. Moreover, it was found that the oxidation process is irreversible: the spin-orbit transition signal does not recover upon the removal of adsorbed oxygen species. Work in progress to track the catalytic activity of these adsorbed $O_2$ species and spin-orbit transition by probe molecules suitable for the redox cycle.

O 63.6 Wed 11:45 H25

**Nucleation of TMDAH on CoO nanoislands on Au(111)** — •Jonas Hauner, Nikolai Sidorenko, Hanna Bühlmeyer, and Jörg Libuda — Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Atomic layer deposition (ALD) has recently received considerable attention as a promising method to precisely grow thin films of a wide variety of materials. This work focuses on the ALD of $HfS_2$ on oxide substrates. In specific, we report on the nucleation behavior of the ALD precursor tetrakis(dimethylamido)hafnium(IV) (TMDAH) on cobaltoxide nanoislands on Au(111). The samples were prepared by deposition of Co in oxygen atmosphere and subsequent deposition of TMDAH. We investigated the adsorption of TMDAH by scanning tunneling microscopy (STM) and infrared absorption reflection spectroscopy (IRAS). At 300 K, TMDAH nucleates at OH groups at the CoO surface by means of a Brønsted acid-base reaction. At 400 K, the mechanism changes and involves a Lewis acid-base reaction due to the lack of OH groups on the substrate. Presaturation of the substrate with $H_2O$ further modifies the reaction mechanism of nucleation.

O 63.7 Wed 12:00 H25

**Maghemite ($\gamma$-$Fe_2O_3$): From Bulk Phases to (001) Oriented Surfaces** — •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]International Max Planck Research School on Sustainable Metallurgy, Max-Planck-Straße 1, 40237, Düsseldorf, Germany

Maghemite ($\gamma$-$Fe_2O_3$) finds applications across a wide range of fields, including spintronics, magnetic recording, and nano-medicine, to name a few. It can be derived from the magnetite ($Fe_3O_4$) structure by introducing Fe vacancies in the B layers containing octahedral Fe ions and oxygen. A stoichiometric phase is achieved by tripling the cubic cell along the c-axis, resulting in a charge-transfer insulator with band gap of 1.90 eV. Phonon dispersion indicates that the cubic structure is stable without imaginary frequency modes. *Ab initio* molecular dynamics (AIMD) simulations confirm the stability at 300 K. Additionally, we explore the stability of the (001) surface within the framework of *ab initio* thermodynamics. The A and B layer terminations are favored at oxygen-poor and oxygen-rich conditions, whereas at intermediate oxygen chemical potentials, a 0.5A layer termination is stabilized. While the A termination exhibits only a minor band gap change, a significant decrease occurs for the B-layer termination due to reduction of magnetic moments and Fe-O bonds up to 0.21 Å. These surfaces serve as a starting point to explore the mechanism of hydrogen adsorption and reduction of the material in view of green steel production.

O 63.8 Wed 12:15 H25

**New insights into CO adsorption on $TiO_2$(110): Enhanced IRAS characterisation** — •Nail Barama, Moritz Eder, Igor Sokolović, Michele Reticcioli, David Rath, Michael Schmid, Ulrike Diebold, Jiri Pavelec, and Gareth Parkinson — Institute of Applied Physics, TU Wien, 1050 Vienna, Austria

$TiO_2$(110) serves as a model system for investigating surface reactivity and catalytic behavior, with CO adsorption commonly employed as a probe molecule. While previous IR spectroscopy studies identified two distinct adsorption sites for low coverages, regular Ti sites, and Ti sites near oxygen vacancies[1,2], recent work based on DFT and microscopy suggests the existence of additional adsorption configurations influenced by the polaronic nature of the substrate[3]. In this contribution, we present experimental results obtained using our custom-built reactivity and infrared reflection absorption spectroscopy (IRAS) setup[4]. This design, optimized for detecting small concentrations of adsorbates on metal oxide surfaces, delivers high-resolution spectra with a high signal-to-noise ratio, allowing us to observe new features. Our data reveal multiple CO adsorption configurations on $TiO_2$(110), which agrees with STM observations from a recent study[3]. References: [1] Xu, M. et al. Angew. Chem. Int. Ed. 51, 4731-4734 (2012). [2] Petrik, N. G. & Kimmel, G. A. J. Phys. Chem. Lett. 3, 3425-3430 (2012). [3] Reticcioli, M. et al. Phys. Rev. Lett. 122, 016805 (2019). [4] Rath, D. et al. Rev. Sci. Instrum. 95, 065106 (2024).

## O 64: Focus Session Atomic Scale Investigation of Magnetic 2D Materials

The rapid expansion of the family of magnetic two-dimensional (2D) materials led to the observation of various types of magnetic order in the 2D limit, such as (anti-)ferromagnetism, noncolinear structures, and magnetic moiré effects. On the fundamental level, there are various open questions regarding the mechanisms that underlie these ground states, as well as the understanding of the role of the interface and dimensionality.

Epitaxial growth of 2D magnetic materials on inert substrates under ultrahigh vacuum conditions and respective in situ investigation allows direct and unambiguous comparison between experimental findings and theoretical calculations. Experimentally, (spin-polarized) scanning tunneling microscopy methods are ideal to explore the electronic structure and magnetic properties of emerging 2D magnetic phases with ultimate real-space and energy resolution at low temperatures. These results are often corroborated by averaging techniques such as X-ray magnetic circular dichroism or magneto-optic Kerr effect. Theoretically, the use of model Hamiltonians requires atomically well-defined systems to precisely predict the electronic and magnetic properties. Combining these complementary approaches helps to elucidate the role of the substrate, defects, and the coupling between quasiparticles in stacked heterostructures.

This focus session aims at highlighting recent progress in the growth and characterization of magnetic states in epitaxial 2D materials and 2D heterostructures on metal substrates, bringing together experts from the fields of scanning probe techniques and first-principles calculations. The overall goal of the session is to gain fundamental insights into the driving mechanisms of 2D magnetic phases.

Organized by
Jeison Fischer, University of Cologne, Germany,

Wouter Jolie, University of Cologne, Germany.

Time: Wednesday 15:00–18:00 Location: H2

**Invited Talk** O 64.1 Wed 15:00 H2
**Topological spin structures in two-dimensional van der Waals magnets and heterostructures** — •Stefan Heinze — Institute of Astrophysics and Theoretical Physics, University of Kiel, Germany

Two-dimensional (2D) van der Waals (vdW) magnets offer exciting opportunities for topological magnetism due to high-quality interfaces, the possibility of single-atomic layer systems, and easy control of magnetism via external stimuli [1]. Here, we explore nano- and atomic-scale topological spin structures in 2D vdW magnets and heterostructures based on first-principles calculations and atomistic spin simulations. A focus is given to heterostructures based on the 2D vdW magnet $Fe_3GeTe_2$ which is experimentally accessible and exhibits favorable properties such as a high transition temperature. An essential prerequisite to apply topological spin states such as skyrmions in future applications is a sufficient stability which we quantify by calculating their lifetime using transition-state theory [2,3]. All-electrical skyrmion detection is proposed via the tunneling anisotropic and non-collinear magnetoresistance considering both a scanning tunneling microscopy geometry and a planar tunnel device structure [4]. Finally, the all-magnetic vdW heterostructure $Fe_3GeTe_2/Cr_2Ge_2Te_6$ is studied and the stability of bimerons in $Cr_2Ge_2Te_6$ is discussed [5].
[1] Q. H. Wang *et al.*, ACS Nano **16**, 6960 (2022).
[2] D. Li *et al.*, Nano Lett. **22**, 7706 (2022).
[3] D. Li *et al.*, Phys. Rev. B **109**, L220404 (2024).
[4] D. Li *et al.*, Nano Lett. **24**, 2496 (2024).
[5] D. Li *et al.*, arxiv: 2408.15974 (2024).

**Invited Talk** O 64.2 Wed 15:30 H2
**Ferromagnetic Order in 2D Layers of Transition Metal Dichlorides** — Andrea Aguirre[1], Andres Pinar[2], Diego Soler[2], Carmen Gonzalez-Orellana[1], Jon Ortuzar[3], Oleksandr Stesovych[2], Celia Rogero[1], Jose Ignacio Pascual[3], Pavel Jelinek[2], Maxim Ilyn[1], and •Martina Corso[1] — [1]Centro de Fisica de Materiales, San Sebastian, Spain — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [3]CIC NanoGUNE, San Sebastian, Spain

Transition metals dihalides are an ideal class of van der Waals materials that enable the study of magnetic phases as function of the transition metal and halide composition as predicted by theory. Here, we characterize the magnetic and electronic properties of 2D magnets based on metallic dichlorides. The materials form flat epitaxial layers on Au(111) with semiconducting character. By X-Ray Magnetic Circular Dichroism (XMCD) measurements we find that single layers of FeCl2 and NiCl2 are soft ferromagnets on Au(111) and their magnetization can be switched from out-of-plane to in-plane by substituting the metal ion from Fe to Ni. Using low temperature scanning tunnelling microscopy with tips functionalized with a nickelocene molecule as magnetic sensor, we confirm the magnetic order of the materials at the atomic scale even at zero applied magnetic field. We thus established a correlation between the mesoscopic magnetic properties probed by XMCD and the atomic spins. Our results suggest that these 2D semiconducting magnets could be implemented in van der Waals heterostructures for applications in spintronics and opto-spintronics.

**Invited Talk** O 64.3 Wed 16:00 H2
**Tailoring spin lattice in van der Waals monolayer crystals** — •Ying-Shuang Fu — Huazhong University of Science and Technology, Wuhan, Chinaina

Spin lattices in monolayer van der Waals (vdW) crystals provide a paradigm for exploring both fundamental spin physics at the 2D limit and miniaturized spintronic applications. Here, we present our recent research in the construction of spin lattices with molecular beam epitaxy and addressing their spin states with both spin-averaged and spin-polarized scanning tunneling microscopy. We explored artificial Kondo lattices in monolayer vdW crystals aiming to emulate protocol heavy fermion systems. We realized quasi-1D Kondo lattice in monolayer stripe-phase 1T-NbSe2 and superconducting 2D Kondo lattice in monolayer VSe2 grown on NbSe2. We also investigated intrinsic magnetic order in monolayer vdW crystals using spin-polarized scanning tunneling microscopy. We identified an antiferromagnetic order in monolayer CrTe2, unraveling the indispensable role of interlayer coupling in determining the magnetic order. Based on that finding, we further fabricated Janus CrTeSe monolayer, and regulates the magnetic anisotropy energy via the symmetry breaking introduced from the Janus structure. Our study resolves intrinsic magnetism with atomic-scale resolution down to monolayer limit, opening up an avenue for studying the unusual spin excitations.

**Invited Talk** O 64.4 Wed 16:30 H2
**Spin excitations in 2D heterostructures from realistic fermionic models** — •António Costa — Center of Physics of the University of Minho, Braga, Portugal — International Iberian Nanotechnology Laboratory

Spin excitations dominate the magnetic response of ferromagnetic two-dimensional crystals. The interplay between low dimensionality, reduced symmetry and spin-orbit coupling endows spin excitations in those materials with intriguing properties, such as non-trivial topology and non-reciprocity. Moreover, spin-orbit coupling connects spin and charge degrees of freedom, opening up paths to electrical control and detection of magnetic states. I will present a microscopic description of the spin response of nanostructured materials based on Hamiltonians for itinerant fermions, derived from DFT calculations. This approach incorporates spin-orbit coupling, does not rely on postulated spin models, and can be applied to insulating or conducting 2D heterostructures, with any kind of magnetic order. I will discuss the properties of magnons in insulating and metallic van der Waals ferromagnets, as well as in 2D molecular crystals. I will also discuss the proximity effect in a heterostructure formed by a 2D ferromagnet and graphene.

O 64.5 Wed 17:00 H2
**Monolayer Multiferroic - Superconductor van der Waals Heterostructures** — •Büşra Gamze Arslan, Mohammad Amini, Ziying Wang, Robert Drost, and Peter Liljeroth — Department of Applied Physics, Aalto University, P.O. Box 15100, 00076 Aalto, Espoo, Finland

Topological superconductivity, a quantum phase hosting robust edge modes like Majorana zero modes (MZMs), holds promise for fault-tolerant quantum computation due to its stability against disturbances. Stacked van der Waals materials offer a promising platform to engineer topological superconductors, as they arise from the interactions between superconductors and magnetic materials. With its helical magnetic order and intrinsic spin-orbit coupling, multiferroic $NiI_2$ is an excellent component for heterostructures realising topological superconductivity.

Here we present our study on monolayer $NiI_2$ grown on superconducting bulk $NbSe_2$. This system is characterized using scanning tunneling microscopy (STM) and spectroscopy (STS). The effect of doping due to the growth of $NiI_2$ on different substrates is investigated. Our observations revealed that $NiI_2$ does not show ferroelectricity, likely due to the charge transfer from the $NbSe_2$ substrate. In addition, we have investigated the edges of the $NiI_2$ islands, where we found clear signatures of edge modes in the $NiI_2/NbSe_2$ system. Whether these arise from topological effects remains to be seen in future studies. Our results show that combining 2D materials can create custom materials with relevant properties.

O 64.6 Wed 17:15 H2
**Engineering the electronic and magnetic properties of $MPS_3$ (M=Fe, Ni, Co, Mn) materials through alkali metal doping** — Jonah Nitschke[1], •Preeti Bhumla[2], Till Willershausen[1], Patrick Merisescu[3], Lasse Sternemann[1], Valentin Mischke[1], Michele Capra[1], Mira Arndt[1], David Janas[1], Giovanni Zamborlini[4], Silvana Botti[2], and Mirko Cinchetti[1] — [1]TU Dortmund — [2]Research Center Future Energy Materials and Systems, ICAMS, Ruhr University Bochum — [3]University of Bath — [4]Universität Graz

Transition metal phosphorus trichalcogenides, $MPX_3$ (where M represents a transition metal and X represents a chalcogen), have emerged as promising candidates for exploring two-dimensional (2D) magnetism. In this study, we focus particularly on $MPS_3$ (M = Fe, Ni, Co, Mn) materials, both above and below the Néel temperature TN. We investigate the electronic and magnetic properties of these materials using micrometer-scale angle-resolved photoelectron spectroscopy (ARPES) and density functional theory (DFT+U) calculations. We observe an increase in the band gaps and shifts in the M d and S p states below TN in the antiferromagnetic (AFM) phase. The density of states reveals the orbital character of the observed bands, and the strong hybridization between the M d and S p orbitals suggests that the superexchange mechanism, in which the S atom mediates the magnetic interaction between neighboring M ions, is relevant for these materials. Further, we examine the effect of alkali metal doping on the magnetic properties of these transition metal phosphorus trichalcogenides.

O 64.7 Wed 17:30 H2

**Conflicting magnetic anisotropy in 2D metal-organic networks** — •Diego Radillo[1,2], Céline Hensky[1,2], Quy Hien Le[1,2], Manfred Parschau[3], Egzona Isufi Neziri[3], Christian Wäckerlin[1,2], and Pierluigi Gargiani[4] — [1]EPFL, Switzerland — [2]PSI, Switzerland — [3]Empa, Switzerland — [4]ALBA, Spain

This talk presents insights into the properties of 2D metal-organic coordination networks embedded with atoms of conflicting magnetic anisotropies. In particular, we look into the coordination networks of tetracyanoethylene with Ni atoms (NiTCNE), Fe atoms (FeTCNE) and a mixture of both (NiFeTCNE), on a gold(111) surface. NiTCNE is known to be a ferromagnet with an out-of-plane easy axis of magnetization. Whereas, for the conflicting in-plane ferromagnet, we propose FeTCNE as a suitable candidate. In our mixed-network experiments, where the magnetic exchange energy enforces that the preferences of the two metal ions cannot be perfectly satisfied, we observe that the magnetization along the out-of-plane and in-plane axes at the Ni and Fe centers mutually influence each other in a rather rational way. This interaction suggests the potential for fine-tuning the magnetization axis and highlights the importance of investigating spin alignment at the per-atom scale. Scanning probe microscopy (SPM) and non-contact atomic force microscopy (AFM) are employed to inspect the morphology of the networks, while X-ray absorption spectroscopy (XAS) and X-ray mag- netic circular dichroism (XMCD) were utilized to analyze the magnetic properties.

O 64.8 Wed 17:45 H2

**Non-van der Waals 2D Materials: Magnetic State Control** — •Tom Barnowsky[1,2] and Rico Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Duke University, Durham, USA

Non-van der Waals (non-vdW) 2D materials – exfoliated from non-layered bulk structures [1] – offer unique opportunities for exploring magnetic properties and their surface-assisted manipulation.

In recent data-driven studies [2,3], we predict several dozen exfoliable candidates. Many of these materials exhibit intrinsic magnetism, notably due to magnetic surface cations, which lead to strong surface spin polarization. Furthermore, the exposed "dangling" bonds at their surfaces – created by bond breaking during exfoliation from the bulk – enable passivation that can significantly modify their electronic and magnetic properties [4]. This passivation-based tuning can, for example, switch the magnetic state of these materials, *i.e.*, alter their local spin symmetry. Most notably, non-vdW 2D $CdTiO_3$ – a diamagnetic compound in its pristine form – becomes ferromagnetic upon hydrogenation. Using data mining and autonomous density functional theory, we demonstrate the potential of these materials as a powerful platform for magnetic state control, opening new possibilities for spintronics.

[1] A. Puthirath Balan *et al.*, Nat. Nanotechnol. **13**, 602 (2018).
[2] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[3] T. Barnowsky *et al.*, Adv. Electron. Mater. **9**, 2201112 (2023).
[4] T. Barnowsky *et al.*, Nano Lett. **24**, 3874 (2024).

## O 65: Solid-Liquid Interfaces: Reactions and Electrochemistry III

Time: Wednesday 15:00–17:45 Location: H6

O 65.1 Wed 15:00 H6

**Potential Pulsed CO2 Reduction Reaction on Polycrystalline Copper Electrodes Studied with Operando Plasmonic Interface Analysis** — •Hagen Übele, Katharina Krischer, and Moritz Josef Feil — Chemische Physik fern des Gleichgewichts Technische Universität München, München, Deutschland

This contribution highlights the use of polished polycrystalline Cu electrodes for the CO2 reduction reaction. By applying time-periodic potential pulses, long-term stability and enhanced selectivity towards hydrocarbon products like methane, ethylene, and ethanol are achieved. These methods rival the performance of nano-structured oxide-derived catalysts or Cu single crystal electrodes while improving electrode longevity.

Operando monitoring is conducted using a plasmonic interface analysis technique with a time resolution of 100 ms. This enables real-time tracking of the Cu oxidation state and the nano-morphology of the electrode surface during potential pulses. The study demonstrates that optimized pulsing protocols can significantly extend the stability of Cu electrodes without the need for pre-manufactured nanostructures.

O 65.2 Wed 15:15 H6

**Au(111) in the Ionic Liquid [MPPip][TFSI]: Corrosion, Reconstruction and Other Surface Restructuring Phenomena** — •Maren-Kathrin Heubach[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.

In fundamental electrochemistry, Au single-crystals are a good benchmarking standard because of the ease of their preparation and high chemical stability.[1-4] Nevertheless, the morphological stability of Au under measurement conditions is rather limited. In this study, we utilize *in situ* scanning tunnelling microscopy (STM) to investigate the stability of a Au(111) electrode in the ionic liquid *N*-methyl-*N*-propylpiperidinium bis(trifluoromethane)sulfonimide ([MPPip][TFSI]). We will provide an overview of the observed surface structures and the corresponding potential ranges in which they remain stable.

[1] J. M. Hermann, *et al.* Electrochim Acta 2020, 347, 136287. [2] M.-K. Heubach, *et al.* ChemElectroChem 2022, 9, e202200722. [3] X. Hu, *et al.* Sci. Bull. (Beijing) 2015, 60, 877-883. [4] L. A. Kibler, *et al.* in Encyclopedia of Solid-Liquid Interfaces, Elsevier, 2024, pp. 426-449.

O 65.3 Wed 15:30 H6

**The relationship between composition, structure and activity of well-defined Pt-Ru alloys during electroreduction of acetone** — •Robert Hübsch[1], Pankaj Kumar Samal[2], Frederike Jäschke[1], Tomáš Skála[2], Nataliya Tsud[2], Josef Mysliveček[2], Olaf Brummel[1], Yaroslava Lykhach[1], and Jörg Libuda[1] — [1]Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Department of Surface and Plasma Science, Charles University, Prague, Czech Republic

The isopropanol/acetone couple can be used as an electrochemically active liquid organic hydrogen carrier (EC-LOHC). PtRu-based alloys are the state-of-the-art catalysts for the electrooxidation of isopropanol. We have investigated the reverse reaction, i.e. electrochemical reduction of acetone, on well-defined PtxRu1-x alloys by means of cyclic voltammetry (CV), synchrotron radiation photoelectron spectroscopy (SRPES) coupled with an ex-situ emersion electrochemical cell, electrochemical infrared reflection absorption spectroscopy (EC-IRRAS), and differential electrochemical mass spectrometry (DEMS). In a systematic study, we established structure-activity relationships for well-ordered PtxRu1-x alloys and surfaces subjected to dealloying in pure and acetone-containing electrolyte. We found that the active state of the catalyst corresponds to the presence of ultra-small Pt aggregates supported on partially oxidized Ru(0001). While Pt(110) forms propane as reduction product, the dealloyed catalysts form the target product isopropanol and suppress propane formation.

O 65.4 Wed 15:45 H6

**Electrochemical XPS for probing the electrified solid-liquid interface of tungsten carbide** — Christoph Griesser, Toni Moser, Sergio Diaz-Coello, and •Julia Kunze-Liebhäuser — Institute of Physical Chemistry, University of Innsbruck, Innsbruck, Austria

A profound understanding of the solid/liquid interface is central in electrochemistry and electrocatalysis, as the interfacial properties determine the electro-reactivity of the system. This study reveals the in-situ surface chemistry evolution of tungsten carbide (WC) powders during electrochemical polarization. WC is known for its platinum-like properties and its high activity towards the hydrogen evolution reaction (HER), but prone to passivation upon air or electrolyte exposure. It is found that the unpreventable surface passivation layer on WC dissolves into the electrolyte under HER conditions, which explains the typically measured high HER electrocatalytic activity of this compound material. The electrochemical (EC-)XPS data provide profound chemical understanding of the electrode/electrolyte interface during operation. This enables fundamental contribution to bottom-up electrocatalyst development, and thus to the advancement of energy conversion and storage technologies.

We thank the FWF for financial support within the Cluster of Excellence MECS.

O 65.5 Wed 16:00 H6

**Degradation of $TiO_2$/Pt catalyst interfaces during operation** — •Sergej Levashov[1], Tim Rieth[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]TUM School of Natural Sciences — [2]Walter Schottky Institut

Photoelectrochemical (PEC) water splitting is a promising approach for generating green fuels. However, photosystems often degrade in the harsh chemical environment required for PEC water splitting. To overcome this limitation, understanding the starting point of the degradation and the exact degradation mechanism at the nanoscale is required. In this work, we study $TiO_2$ thin films grown by atomic layer deposition (ALD) combined with Pt catalyst layers, deposited by sputtering and two different ALD processes, by in-situ/operando atomic force microscopy and elucidate their changes in topography and mechanical properties under operation conditions. The main difference between the Pt is the growth mechanics: while sputtering yields a continuous film, the ALD growth results in Pt islands. On the macroscale, the ALD grown Pt catalysts show similar onset potentials and saturation current densities as the sputtered ones. At the nanoscale, we observe that the ALD Pt films are more stable than sputtered Pt under operation conditions. Complementary, we performed X-ray photoelectron spectroscopy (XPS) before and after PEC operation to reveal chemical changes. Overall, ALD grown Pt catalysts improve the system performance compared to sputtered Pt. These measurements provide important insights into the underlying reaction mechanism and the role of surface restructuring and delamination of catalyst interfaces.

O 65.6 Wed 16:15 H6

**TiO2 passivation of GaInP(100) surfaces** — •David Ostheimer[1], Julius Kühne[2,3], Sahar Shekarabi[1], Agnieszka Paszuk[1], Mohammad Amin Zare Pour[1], Ian D. Sharp[2,3], Wolfram Jägermann[4], and Thomas Hannappel[1] — [1]TU Ilmenau, Inst. of Physics, Fundamentals of Energy Materials, Ilmenau, Germany — [2]TU Munich, Walter Schottky Institute, Garching, Germany — [3]TU Munich, Physics Department, TUM School of Nat. Sciences, Garching, Germany — [4]TU Darmstadt, Surface Science Lab, Darmstadt, Germany

GaInP is widely used in III-V-based photoelectrochemical devices as a top photoabsorber or charge-selective contact, achieving high solar-to-fuel conversion efficiencies. To enhance stability under HER conditions, a thin TiO2 protection layer can be applied. This study investigates the electronic structure of the TiO2/GaInP(100) interface. TiO2 was deposited via atomic layer deposition (ALD) on p-type GaInP(100) grown on GaAs(100) substrates. Two surfaces were prepared: a phosphorus-rich (P-rich) (2x1)-like surface transferred contamination-free under ultra-high vacuum (UHV) and a naturally oxidized surface. X-ray and UV photoelectron spectroscopy revealed a slightly thinner interfacial oxide in the UHV-transferred sample. Initial ALD cycles formed an oxide nearly stoichiometric to the native oxide, but both samples exhibited strong Fermi level pinning, resulting in similar band alignments. These findings highlight the influence of initial oxides on interface control in III-V semiconductors.

O 65.7 Wed 16:30 H6

**Influence of pH and Electrolyte Flow on the Oxidation of Ni anodes at High Overpotentials** — •Justus Leist[1], Timo Jacob[1,2,3], and Albert K. Engstfeld[1] — [1]Institute of Electrochemistry, Ulm, Germany — [2]Helmholtz-Institute-Ulm (HIU), Ulm, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

The electrocalalytic splitting of aqueous electrolytes is typically impeded by the sluggish kinetics of the oxygen evolution reaction (OER). Ni-based catalysts are considered as cost-effective alternatives to the currently used rare metal oxides, such as Ir or Ru. While the fundamental properties of Ni have been studied intensively usually at or around the onset potential for the OER, here we study the OER activity at high overpotentials, which are more closely related to application.

The OER characteristics are studied by means of cyclic voltammetry and polarization curves using Ni electrodes in alkaline solutions. Depending on the experimental conditions, electrolyte pH and flow, the current voltage traces show several features at high overpotentials, which can be attributed to the pH-dependent change in OER kinetics. Based on additional in-situ Raman spectroscopy and electrochemical quartz crystal microbalance measurements we discuss possible structures formed and the degradation of the Ni electrodes under these conditions.

O 65.8 Wed 16:45 H6

**DFT Study of Aldehyde Oxidation and Hydrogen Evolution on Flat and Stepped Gold Surfaces** — •Samuel Mattoso[1], Stefan Wipperman[1,2], Mira Todorova[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237 Düsseldorf — [2]Philipps-Universität Marburg, Renthof 5, Marburg, 35032, Germany

Significant investments are being made in the development of greener industrial processes, with heterogeneous electrocatalysis playing a major role. Gold is known as a catalyst, which selectively oxidizes aldehydes to carboxylic acid. It may also catalyze the hydrogen evolution reaction (HER). These chemical reactions take place at the solid-liquid interface, where the role of step sites, pH, adsorption of intermediates, solvation and applied bias are largely unknown but may be relevant to understand in order to improve performance. We employ DFT simulations to provide mechanistic insights into this system, by probing the interaction of Au(111) and Au(331) surfaces with H, OH and acetaldehyde. The adsorption energies and work function changes as a function of H and OH coverage for different observed patterns will be reported for the two surfaces. In addition, we find that surface imperfections such as step edges are essential for the HER and aldehyde oxidation to proceed, as they dissociatively bind the aldehyde, leading to adsorbed H.

O 65.9 Wed 17:00 H6

**On the pH-dependence of the $H_{upd}$ peak in cyclic voltammograms of Pt-group nanoparticles** — •Hedda Oschinski[1,2], Simeon Beinlich[1,2], Karsten Reuter[1,2], and Nicolas Hörmann[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Technische Universität München, München

Understanding the electrochemical behavior of hydrogen adsorption at Pt-group metal surfaces, particularly in the context of non-well-defined nanoparticle surfaces, is crucial for advancing electrocatalytic applications such as the hydrogen evolution reaction (HER). To this end, we provide insights into the non-Nernstian pH shifts observed for underpotential deposited $H_{upd}$-like cyclic voltammetry (CV) peaks on Pt, Ir, Pd, and Rh nanoparticles. Utilizing density-functional theory, we explore the potential-dependent stability of H and OH adsorbates at undercoordinated surface sites, emphasizing the role of non-ideal electrosorption valencies in these shifts. This identifies direct H-OH replacement as predominant mechanism behind the CV peaks and reveals a primary influence of partial charge transfer. The theoretical predictions show good agreement with experimental observations across various Pt-group metals, even over various surface coordinations, and provide insights into cation-specific effects at Pt across the entire pH scale. This work not only clarifies the origin of the $H_{upd}$-like peak shift within the water stability region, but also suggests the interfacial capacitance as a main descriptor for cation effects in the HER, paving the way for more detailed analyses of cation type, concentration, and interfacial solvent structure.

O 65.10 Wed 17:15 H6

**From model to realistic copper sulfide electrocatalyst** — •Roser Fernandez Climent, Jesus Redondo, and Martin Setvín — Charles University, Prague, Czech Republic

Copper sulfide is a widely studied material in electrocatalysis. In this study, we synthesized copper sulfide thin films electrochemically under inert conditions, enabling precise control of material properties and minimizing contamination risks. The films were transferred in-vacuum for surface characterization using X-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED), and scanning transmission electron microscopy (STEM).

O 65.11 Wed 17:30 H6

**Stability of Pd-Rh core-shell electrocatalysts supported on Co3O4(111) in alkaline environment** — Alexander Simanenko[1], Jan Škvára[2], Pankaj Kumar Samal[2], Evanie Franz[1], Robert Hübsch[1], Tomáš Skála[2], Nataliya Tsud[2], Sascha Mehl[3], Viktor Johánek[2], Josef Mysliveček[2], Olaf Brummel[1], •Yaroslava Lykhach[1], and Jörg Libuda[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Charles University, Prague, Czech Republic — [3]Elettra-Sincrotrone Trieste SCpA, Basovizza-Trieste, Italy

The electronic metal-support interaction (EMSI) is considered as an efficient strategy to stabilize the noble metal nanoparticles against sintering, but its consequences under the electrochemical conditions remain elusive. We investigated the effect of the EMSI on the stability of bimetallic Pd@Rh and Rh@Pd core@shell nanoparticles supported on well-ordered Co3O4(111) films in alkaline electrochemical environment by means of synchrotron radiation photoelectron spectroscopy (SRPES) coupled with ex-situ emersion electrochemical cell. We found that the EMSI promotes strong oxidation of Rh metal. The extent of Rh oxidation strongly depends on the specific metal/oxide interface configuration below the core@shell nanoparticles. Our study suggests that decoupling the Rh metal and the Co3O4(111) substrate by constructing the Pd/Co3O4(111) interface below Pd@Rh core@shell nanoparticles reduces the effect of the EMSI and improves the stability of the electrocatalyst toward oxidation.

## O 66: Vacuum Science Technology: Theory and Applications

Time: Wednesday 15:00–18:00 Location: H8

**Invited Talk** O 66.1 Wed 15:00 H8

**Unveiling the crucial role of kinetic modeling of gas flows in vacuum and fusion technologies** — •Christos Tantos and Thomas Giegerich — Institute for Technical Physics, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, 76344, Germany

Accurate and reliable modeling of non-equilibrium flows is not only of academic interest within the scientific community, including the field of vacuum gas dynamics, but is also crucial for the design and enhancement of engineering processes, such as those in vacuum and fusion technologies. In these applications, the flow is characterized by molecular mean free paths that are comparable to the reference characteristic length, making a particle-based description of the flow field essential. This requires the use of the Boltzmann equation and widely accepted numerical methods for solving it, such as the stochastic Direct Simulation Monte Carlo (DSMC) and the deterministic Discrete Velocity Method (DVM).

This talk discusses key aspects of rarefied gas dynamics in vacuum and fusion technologies, emphasizing the link between theory and practice. It is divided into two parts. The first covers recent advances in modeling multicomponent transport phenomena in vacuum technology using DSMC and DVM methods, with a focus on gas separation in multicomponent flows. The second part analyzes vacuum gas dynamics in fusion systems, presenting numerical simulations (2D and 3D) of pumping systems in fusion machines and highlighting their design impact.

**Invited Talk** O 66.2 Wed 15:30 H8

**Advances in traceable vacuum and outgassing rate measurements** — •Matthias Bernien[1], Annas Bin Ali[1], Thomas Bock[1], Tom Rubin[1], Janez Setina[2], Perrin Waldock[3], Kirk Madison[3], and Karl Jousten[1] — [1]PTB, Abbestr. 2-12, 10587 Berlin — [2]IMT, Lepi pot 11, 1000 Ljubljana, Slovenia — [3]University of British Columbia, 6224 Agricultural Road, Vancouver, B.C. V6T 1Z1, Canada

For the pressure range from 10 mPa to 130 Pa, a fully automated static expansion system made of aluminum has been set up and validated. Its principle involves transferring a fixed amount of gas from a smaller volume to a larger one, creating a well-defined lower pressure, provided that the initial pressure and the volume ratio are accurately known. Relative standard measurement uncertainties between 0.08% and 0.012% are achieved. Primary standards utilizing cold atom traps offer a promising new approach for realizing the pascal in the UHV range by measuring the loss rate caused by collisions with gas molecules. To establish these standards, the University of British Columbia and PTB have carried out a comparison between a mobile standard based on cold atoms and a continuous expansion system for $N_2$, Ar and $H_2$. In the semiconductor industry, outgassing from components in vacuum must be well controlled. Contaminants are monitored using QMSs which lack stability. This is particularly problematic when maximum levels of contaminants must be agreed between manufacturers and suppliers. To improve the comparability of outgassing rate measurements, reference samples for dodecane and water have been developed suitable for in-situ calibration of QMSs.

O 66.3 Wed 16:00 H8

**BeamPipes4ET: Innovative On-Site Production and Welding of the Einstein Telescope Vacuum Tubes** — Charlotte Benning, •Robert Joppe, Oliver Pooth, and Achim Stahl — III. Physikalisches Institut B, RWTH Aachen

The Einstein Telescope will be the first gravitational wave detector of the third generation. It requires about 120 km of vacuum tubes with a diameter of 1 m to achieve the design sensitivity and reduce scattered light. BeamPipes4ET introduces an innovative production concept for vacuum pipes, incorporating a new welding technology and adapting existing flange and T-section production methods. This approach enhances reliability, significantly reduces labor, welding, and finishing efforts. By manufacturing pipes on-site from coils of sheet metal in a continuous process, transportation needs are minimized, and pipe connections are eliminated. Additionally, the project pioneers laser beam welding under mobile vacuum and transfers advanced pipe feature integration technologies to further streamline production.

This talk presents the current status and ongoing activities in the BeamPipes4ET project.

O 66.4 Wed 16:15 H8

**Aluminum fiber optical vacuum feedthroughs for challenging environments** — •Christoph Bartlitz, Kristian Kirsch, Marco John, Marcel Hannemann, Andreas Trützschler, and Klaus Bergner — VACOM Vakuum Komponenten & Messtechnik GmbH, In den Brückenäckern 3, 07751 Großlöbichau, Germany

Fiber optical components are used in a wide variety of places, both in scientific experiments and in production processes in vacuum systems. In principle, these components enable interference-free transmission of the finest measurement signals over long distances, robust sensor technology and maximum transmission speed. Hermetic optical fiber feedthroughs based on stainless steel, ceramics and quartz glass have become established for coupling light signals to vacuum- and process chambers.

We designed and tested a novel optical fiber feedthrough whose metallic components are made entirely of aluminum.

These technologies enable the application of optical fibers as in-vacuum diagnostic within challenging environments. Thereby, the diagnostic is driven by fiber Bragg gratings (FBGs) in the optical fiber itself. The application of FBGs as an in-vacuum temperature sensor is demonstrated, where an optical fiber containing a bunch of several FBGs becomes a compact, stable, robust, and flexible network of local sensors at different positions in vacuum with up to km-length signal path.

O 66.5 Wed 16:30 H8

**Comparative Measurements of Ion Pump pumping speed according to ISO/DIS 3556 and DIN 28429** — •Marcel Herrmann, Kristian Kirsch, Marco John, Christoph Bartlitz, Andreas Trützschler, and Klaus Bergner — VACOM Vakuum Komponenten & Messtechnik GmbH, In den Brückenäckern 3, 07751 Großlöbichau

Sputter Ion Pumps (SIP) offer an appealing strategy to efficiently maintain ultra-high and extremely-high vacuum conditions in a vacuum chamber. The pumping speed, i.e. the volume flow of gas extracted from the vacuum in a specific period of time, can be determined according to various standards. However, recorded pumping speeds may vary severely, depending on the standard chosen and the detailed procedure applied. This talk compares experimentally obtained pumping speeds of several SIPs, acquired according to the most commonly applied standards, DIN 28429:2014 05 and ISO/DIS 3556 1.2(1992).

O 66.6 Wed 16:45 H8

**Performance and future of the KATRIN experiment after 6 years of tritium operation** — •Joachim Wolf — Karlsruher Institut für Technologie (for the KATRIN Collaboration)

The Karlsruhe Tritium Neutrino experiment (KATRIN) searches for the effective electron neutrino mass with electrons from the $\beta$-decay of tritium with an unprecedented sensitivity of <0.3 eV/c2. The $\beta$-electrons are guided magnetically through the 70-m long setup, moving from the gaseous tritium source through a differential pumping section (DPS) and a cryogenic pumping section (CPS) to the high-resolution spectrometer. In the spectrometer, the kinetic energies of the decay electrons are analysed in an electrostatic high-pass filter (MAC-E-filter). Background considerations require a very good vacuum in the order of 10-11 mbar in the large spectrometer vessel (volume 1240 $m^3$, surface: 1222 $m^2$). A combination of NEG pumps and turbo-molecular pumps reliably provides the necessary pumping speed since more than 10 years. In addition, a very clean surface and low outgassing rates are mandatory.

After several years of engineering runs, the experiment started full tritium operation in March 2019, searching for the effective mass of electron-anti-neutrinos. These measurements will finally end in December 2025, followed by hardware upgrades and a new physics program. This talk reports on the performance of the components, after almost 20 years of R&D and 6 years of tritium operation with special emphasis on vacuum-related issues, followed by a description of future plans for the KATRIN setup.

O 66.7 Wed 17:00 H8

**Miniaturized Pirani vacuum sensor with active heat-loss compensation** — •Julian Eiler[1], Stefan Weber[2], Peter Gerlesberger[2], Heinz Plöchinger[2], and Rupert Schreiner[1] — [1]Faculty of Applied Natural Sciences and Cultural Studies, OTH Regensburg, D-93053 Regensburg, Germany — [2]Thyracont Vacuum Instruments GmbH, D-94036 Passau, Germany

Pirani sensors measure the thermal conductivity of the residual gas in a vacuum by creating a thermal gradient between a heated sensor element and a heat sink. The heat flux from the sensor element to the heat sink over the residual gas is a measure of the vacuum and can be determined by the electrical power applied.

In addition to the heat flux over the gas, there are further energy losses from the heating structure due to radiation and parasitic heat fluxes via the suspensions of the sensor element. These losses reduce the sensitivity of the sensor.

For this reason, a Micro-Pirani sensor in the shape of a microhotplate was developed that actively compensates the heat flux via the suspensions. This was achieved by placing additional heating structures on the suspensions, which interrupt the heat flow from the sensor element via the suspensions during operation. This active compensation improves the sensitivity at low pressures, enabling vacuum measurements from atmospheric pressure down to 10e-6 mbar.

O 66.8 Wed 17:15 H8

**Feasibility Study on Laser-Based Real-Time Monitoring of Hydrogen Atom Beams** — •Tobias Geier, Alexander Marsteller, and Robin Grössle — Karlsruher Institute for Technology, IAP-TLK, for the KAMATE Collaboration

Through the observation of neutrino oscillations, it has been shown that there are three different neutrino mass eigenstates. Current measurements of the oscillation length of the flavor states yield a lower limit for the effective electron neutrino mass of $\sim 0.05$ eV (inverted ordering) or $\sim 0.01$ eV (normal ordering). The sensitivity of the KATRIN experiment is limited to $\sim 0.3$ eV. Therefore, future experiments which aspire to achieve inverted ordering or better need new technologies. For the next generation of experiments aiming at the direct determination of the neutrino mass using high-resolution beta spectroscopy on tritium, atomic tritium is to be used. The advantage over the currently used molecular tritium ($T_2$) lies in the avoidance of molecular excitations in the $^3HeT^+$ daughter molecule, which lead to a smearing of the beta spectrum, thus limiting the maximum achievable resolution. In order to employ atomic tritium for beta spectroscopy, it is essential to cool it to a few mK and trap it magnetically. A method for contactless real-time analysis of the beam is required to monitor and control the operation of the atomic source. This talk presents a method for characterizing the beam profile based on Rayleigh scattering of a laser beam. By measuring the intensity with a sensitive camera, the particle density can be mapped. In this contribution, the results of a first experimental feasibility study are presented.

O 66.9 Wed 17:30 H8

**Challenging tasks in modern vacuum technology applications** — •Kristian Kirsch, Andreas Trützschler, Christoph Bartlitz, Marcel Herrmann, Marco John, and Klaus Bergner — VACOM Vakuum Komponenten & Messtechnik GmbH In den Brückenäckern 3 07751 Großlöbichau / Germany

Cutting-edge technology from the field of particle accelerators, quantum technology applications and lithography is pushing the limits of vacuum technology. In general, off-the-self' products are not sufficient for that. In this context, product developers and scientists need to find a joint language to deal with this task. The focus of this talk is to explain needs and challenges of today's cutting edge technology applications related to vacuum requirements. Therefore, we address different state-of-the-art applications. One focus is the fundamental difficulty to fulfill demanding vacuum conditions in one compact system. On the other hand, we address the complex and demanding task of isolating quantum objects within a quantum application like quantum computing, quantum gravimetry, and quantum metrology. Based on this, benefits and drawbacks of different vacuum technology solutions to all of these requirements are shown within the transition from customized single components to standardized and industrial ready serial components.

O 66.10 Wed 17:45 H8

**Different Approaches to Vacuum System Performance Improvement for the Einstein Telescope** — •Charlotte Benning, Robert Joppe, Maike Kühler, Stefan Krischer, Oliver Pooth, and Achim Stahl — III. Physikalisches Insitut B, RWTH Aachen

The Einstein Telescope will be the next European gravitational wave detector. It requires about 120 km of vacuum tubes in tunnels with a diameter of 1 m for a laser beam to achieve the design sensitivity. The required pressure of less than $10^{-11}$ mbar introduces the need for innovations that help with performance improvement and cost reduction. The current baseline concept of the vacuum system includes passive sections of stainless steel welded inside the tunnels and connected to pumping stations. Achieving ultra-high vacuum (UHV) in these tubes requires high pumping capacities and long bake-out times of the tubes, which are associated with high energy and equipment costs.

This talk discusses two possible improvements over the baseline design: Integrating non-evaporable getter (NEG) surfaces into the inside of the tubes to reduce costs and aiming for a more homogeneous distribution of pumping power (distributed pumping). Furthermore, forming seamless flanges from the pipe material eliminating the need for welding is presented, which is especially relevant for the underground environment of the Einstein Telescope.

# O 67: Ultrafast Electron Dynamics II

Time: Wednesday 15:00–17:45 Location: H11

O 67.1 Wed 15:00 H11

**Polaron formation in NiO analysed by transient absorption spectroscopy** — •Mahendra Kabbinahithlu[1], Björn Sothmann[1], Fred Hucht[1], Sergey Kovalenko[2], Tobias Lojewski[1], Nico Rothenbach[1], Katharina Ollefs[1], Heiko Wende[1], Uwe Bovensiepen[1], Julia Stähler[2], and Andrea Eschenlohr[1] — [1]Universität Duisburg-Essen, Fakultät für Physik und Center for Nanointegration (CENIDE), Lotharstraße 1, 47057 Duisburg, Germany — [2]Humboldt-Universität zu Berlin, Institut für Chemie, Brook-Taylor-Straße 2, 12489 Berlin, Germany

Polaron formation is the process by which free electrons in a material find a lower energy localized state by distorting their surrounding lattice. The polaron formation timescales and its fluence dependent dynamics in nickel oxide (NiO) from time-resolved optical absorption studies is discussed here.

NiO is pumped above the band gap with 3.98 eV energy photons, and is probed using a time-delayed supercontinuum. The time-resolved absorption spectrum shows negative ground state bleach and positive excited state absorption and in addition, a time-delayed and energy separated appearance of a positive feature at 3.35 eV that is discussed as the signature of polaron formation. With increasing fluence,the build-up time of this 3.35 eV signature decreases from 4 ps down to 1.1 ps, indicating the transition from isolated polarons to the formation of a polaron band. The spectrally distinct transition between low fluence and high fluence regimes is used to estimate the polaron size and the dynamics is modelled by coupled rate equations.

O 67.2 Wed 15:15 H11

**Sharp Exciton Mott Transition in $WS_2$ and its Ultrafast Decay** — •Subhadra Mohapatra[1], Lukas Gierster[1], Samuel Palato[1], Nicholas Michael Olsen[2], Xiaoyang Zhu[2], and Julia Stähler[1] — [1]Humboldt-Universität zu Berlin, Institut für Chemie — [2]Columbia University

The excitonic Mott transition (EMT) in transition metal dichalcogenides is reported to be either discontinuous [1] or continuous [2]. To resolve the ambiguity, here we study the optical response of $WS_2$ across the Mott density. Using a complex lineshape analysis, we separate the optical response in the photo-excited part of the sample from the unexcited regimes. In agreement with a continuous EMT, a gradual increase in the bleach of the sample-averaged absorption is observed. However, the lineshape analysis unveils a sharp discontinuity in the transient dynamics of the A and B exciton resonances above a critical photoexcitation density. This is attributed to plasma formation followed by band gap renormalization. The plasma decays with a laser fluence-independent time constant of 0.65 ps which is attributed to phase separation into excitonic and plasma regions, in agreement with the literature [3,4]. This work not only provides the first detailed experimental investigation of the EMT close to the critical limit but also highlights the role of spatial inhomogeneous charge carrier distribution for the widely used transient optical spectroscopies of 2D materials. References: [1] Bataller et al. Nano Lett 19(2) (2019). [2] Chernikov et al. Nat Photonics 9(7) (2015). [3] Steinhoff et al. Nat Commun 8 (1) (2017). [4] Koch et al. Physica status solidi (b) 238(3) (2003).

O 67.3 Wed 15:30 H11

**Ultrafast formation of electron polarons in rutile $TiO_2(110)$** — •xiang zhang, lukas gierster, and julia stähler — Humboldt-Universität zu Berlin, Institut für Chemie

The electron dynamics at $TiO_2$ surfaces are widely studied, mainly focusing on the defect-induced electronic states [1,2]. Additionally, recent calculations suggest that upon across-bandgap excitation, electron polarons form within 25 fs by trapping of photoexcited electrons inside the deformed lattice [3]. Using time-resolved photoelectron spectroscopy, we observe the instrument response-limited (<30 fs) rise of a photoinduced electron population at 0.3 eV below $E_F$. To elucidate whether this feature originates from polaron formation, experiments are conducted with different laser fluences, photon en- ergies and under varying surface conditions. Based on this, competing mechanism as exciton formation, surface photovoltage effects and band gap renormalization can be excluded. Our results suggest that photoexcitation of the rutile $TiO_2(110)$ surface creates small sub-surface polarons within only 30 fs.

Reference:
[1] A. Argondizzo et al. J. Phys. Chem. C 120, 12959-12966(2016).
[2] Y. Zhang et al. J. Phys. Chem. Lett. 10, 5265-5270(2019).
[3] C. Gao et al. J. Phys. Chem. C 125, 27275-27282(2021).

O 67.4 Wed 15:45 H11

**Time-resolved two-photon photoemission of antiferromagnetic $LaFeO_3$** — •Friederike Wührl, Antonia Rieche, Anne Oelschläger, Kathrin Dörr, and Wolf Widdra — MLU Halle-Wittenberg

Basic quantities as band gaps or the lifetime of electrons at the conduction band minimum are of strong interest for optoelectronic devives. In this context, strongly correlated oxides are rarely studied. One such example is 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].

We present time-resolved two-photon photoemission (2PPE) data on above band gap excitation of electrons in $LaFeO_3$, a charge-transfer insulator with antiferromagnetic order, which exhibits weak ferromagnetism through spin canting. The band gap opens between hybridized O 2p – Fe $3d_\uparrow$ and minority Fe 3d $t_{2g\downarrow}$ states. Thin films of 9 nm $LaFeO_3$ were prepared on $SrRuO_3/DyScO_3$ substrates using pulsed laser deposition. Low-energy electron diffraction confirmed the formation of single crystalline layers with a c(2x2) superstructure, indicative for the long-range magnetic ordering. In one-colour and two-colour UV-UV pump-probe experiments ($hv = 3.4$ eV and 4.2 eV) we find three unoccupied states at 0.3, 1.3, 2.1 eV above $E_F$, the middle one being resonantly pumped from Fe $e_{g,\uparrow}$ states and exhibiting a short lifetime of 22 fs. At the conduction band minimum we observe a biexponential decay with lifetimes of 40 fs and 1.1 ps.

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

O 67.5 Wed 16:00 H11

**Photo-induced charge-transfer renormalization in NiO** — •T. Lojewski[1], D. Golez[2,3], K. Ollefs[1], L. Le Guyader[4], L. Kämmerer[1], N. Rothenbach[1], R. Y. Engel[5], P. S. Miedema[5], M. Beye[5,6], G. S. Chiuzbaian[7], R. Carley[4], R. Gort[4], B. E. Van Kuiken[4], G. Mercurio[4], J. Schlappa[4], A. Yaroslavtsev[4,8], A. Scherz[4], F. Döring[9], C. David[9], H. Wende[1], U. Bovensiepen[1,10], M. Eckstein[11], P. Werner[12], and A. Eschenlohr[1] — [1]Univ. Duisburg-Essen & CENIDE — [2]Jozef Stefan Inst. — [3]Univ. of Ljubljana — [4]European XFEL — [5]DESY — [6]Stockholm Univ. — [7]Sorbonne Univ. — [8]MAX IV Lab. — [9]PSI — [10]Univ. of Tokyo — [11]Univ. of Hamburg — [12]Univ. of Fribourg

For strongly correlated materials, like the charge transfer insulator NiO, the interplay between the interaction-based localization and the itinerant behaviour of electrons is essential in determining the electronic properties. In these materials, resonant photoexcitations result in convoluted dynamics involving dynamical screening induced band shifts, charge redistributions and *d*-*d* type excitations. By combining fs time-resolved X-ray absorption spectroscopy and dynamical mean-field theory, we disentangle the intertwined dynamics. We find long-lived redshifts of the Ni $L$ and O $K$ edges ($> 10$ ps), arising from a combination of Hartree shifts and renormalization of local interactions. We also identify a short-lived Ni $L_3$ pre-edge feature ($< 1$ ps) related to photo-induced *d*-*d* transitions [1]. Financial support by DFG through SFB 1242 is acknowledged. - [1] T. Lojewski et al., Phys. Rev. B, in press (ArXiv:2305.10145)

O 67.6 Wed 16:15 H11

**Non-equilibrium carrier dynamics and band structure of graphene on 2D silicon** — •Maria-Elisabeth Federl[1], Theresa Glaser[1], Niclas Tilgner[2], Thomas Seyller[2], and Isabella Gierz[1] — [1]University of Regensburg — [2]Technical University Chemnitz

Confinement heteroepitaxy, where novel 2D structures are stabilized at the interface between epitaxial graphene and SiC substrate, provides a pathway to engineer proximity-coupling between the massless carriers in graphene and the carriers in the underlying layer. If the latter is a Mott insulator, exotic electronic properties might emerge due to hybridization between itinerant and localized electrons. The Si-rich (3x3) structure on the surface of SiC(0001) was proposed to be Mott insulating with a bandgap of 1eV [1]. We used confinement heteroepitaxy to prepare a graphene monolayer on top of this putative 2D Mott insulator [2] and searched for indications of interlayer hybridization using time- and angle-resolved photoemission spectroscopy (trARPES). Our findings are consistent with the occurrence of ultrafast charge transfer between graphene and the Si-rich surface structure that we attribute to interlayer hybridization in agreement with predictions from density functional theory [2].

[1] Surf. Sci. 445, 109 (2000)

[2] Phys. Rev. B 94, 245421 (2016)

O 67.7 Wed 16:30 H11

**Direct view on ultrafast charge transfer between C60 molecules and graphene** — •Michael Herb, Maria-Elisabeth Federl, and Isabella Gierz — University of Regensburg

Interfacing 0D molecules with 2D materials holds great potential for various applications in materials science, electronics, and nanotechnology. For example, C60/graphene hybrids have been proposed to serve as supercapacitors or sensitive UV-visible photodetectors. We use time- and angle-resolved photoemission spectroscopy (trARPES) to investigate the interfacial non-equilibrium charge carrier dynamics of a sub-monolayer C60 film deposited on single-layer graphene. Upon excitation below the HOMO-LUMO gap of C60, we observe a shift of the graphene Dirac cone towards higher binding energies and a concurrent shift of the C60 molecular levels towards lower binding energies. These shifts indicate a photoinduced hole doping of graphene that persists for several picoseconds. Based on these findings we propose a possible microscopic pathway for ultrafast charge transfer across the C60-graphene interface.

O 67.8 Wed 16:45 H11

**Light-induced hidden state studied by ultrafast angle-resolved photoemission spectroscopy** — •Junde Liu[1], Pei Liu[3], Liu Yang[3], Sung-Hoon Lee[4], Mojun Pan[2], Famin Chen[2], Jierui Huang[2], Bei Jiang[2], Mingzhe Hu[2], Yuchong Zhang[2], Zhaoyang Xie[3], Gang Wang[3], Mengxue Guan[3], Wei Jiang[3], Huaixin Yang[2], Jianqi Li[2], Chenxia Yun[2], Zhiwei Wang[3], Sheng Meng[2], Yugui Yao[3], Tian Qian[2], and Xun Shi[3] — [1]University of Göttingen, I. Physikalisches Institut, Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [3]Beijing Institute of Technology, Beijing, China — [4]Kyung Hee University, Yongin, Republic of Korea

The non-volatile and ultrafast optical manipulation of material properties offers profound insights into light-matter interactions and holds great potential for optoelectronic applications. However, the discovery of such transitions is often serendipitous, and their practical implementation remains limited, underscoring the need for systematic investigation. In this talk, I will focus on laser-induced nonvolatile phase transitions in transition metal dichalcogenides (TMDs), highlighting the critical role of interlayer order in the formation of hidden states. By employing ultrafast laser excitations (single-pulse writing, pulse-train erasing and pulse-pair control), systematic angle-resolved photoemission spectroscopy (ARPES) characterizations, and comparative density functional theory (DFT) calculations, I aim to unravel the mechanisms that form and stabilize these hidden states, paving the way for novel methods to optically control low-dimensional materials.

O 67.9 Wed 17:00 H11

**A machine-learning approach to understanding ultrafast carrier dynamics in the 3D Brillouin zone of PtBi$_2$** — Paulina Majchrzak[1], Charlotte Sanders[2], Yu Zhang[2], Andrii Kuibarov[3], Oleksandr Suvorov[3], Tami Meyer[1], Gesa Siemann[1], Emma Springate[2], Iryna Kovalchuk[3,4], Saicharan Aswartham[3], Grigory Shipunov[3], Bernd Büchner[3], Sergey Borisenko[3], and •Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, DK — [2]Central Laser Facility, Harwell, UK — [3]IFW Dresden, Germany — [4]Kyiv Academic University, UA

We examine the electron dynamics of the type-I Weyl semimetal PtBi$_2$ by time- and angle-resolved photoemission spectroscopy. By varying the probe photon energy over a wide range, we are able to explore differences throughout the three-dimensional Brillouin zone. For these experiments, the photoemission intensity is measured as a function of emission angle, electron kinetic energy, time delay and probe photon energy. In order to discover trends in this multi-dimensional data set, we apply $k$-means, an unsupervised machine learning technique. This reveals $k_z$-dependent differences in dynamics–in particular, we observe dynamics that are faster in the parts of the Brillouin zone that host most of the bulk Fermi surface than in parts close to the Weyl points.

O 67.10 Wed 17:15 H11

**Tracing thermal and athermal electrons in laser-excited metals** — •Markus Uehlein[1], Henry Snowden[2], Christopher Seibel[1], Tobias Held[1], Sebastian T Weber[1], Reinhard J Maurer[2,3], and Baerbel Rethfeld[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Germany — [2]Department of Chemistry, University of Warwick, United Kingdom — [3]Department of Physics, University of Warwick, United Kingdom

Understanding the energy- and time-resolved electronic properties in metals at the initial athermal stage after femtosecond laser irradiation is of fundamental importance for many applications in surface science. In the time domain, where no electron temperature is defined, the non-equilibrium dynamics are usually described with microscopic methods, such as the Boltzmann equation. However, especially when investigating ballistic transport processes, a description with full Boltzmann collision integrals [1] is challenging due to the numerical effort.

We present a model that describes the athermal carriers efficiently. To that end, we consider thermal and athermal electrons separately. We use a temperature-based approach for the thermal electrons and the phonons, while we trace the distribution of the athermal electrons explicitly. Such a separation allows to conserve particles and energy even when a relaxation time approach is applied. We show the energy-resolved dynamics and find good agreement with time-resolved two-photon photoemission spectroscopy measurements [2].

[1] B. Y. Mueller and B. Rethfeld; Phys. Rev. B **87**, 035139 (2013)

[2] F. Kühne *et al.*; Phys. Rev. Res. **4**, 033239 (2022)

O 67.11 Wed 17:30 H11

**Influence of carbon buffer layer on non-equilibrium carrier dynamics of epitaxial graphene on SiC(0001)** — •Johannes Gradl[1], Leornard Weigl[1], Neeraj Mishra[2,3], Stiven Forti[2], Camilla Coletti[2,3], and Isabella Gierz[1] — [1]University of Regensburg, Germany — [2]Istituto Italiano di Tecnologia, Pisa, Italy — [3]Istituto Italiano di Tecnologia, Genova, Italy

The carbon buffer layer resting at the interface between epitaxial graphene and SiC(0001) substrate is believed to be electronically dead with two non-dispersing bands located well below the Fermi level [1]. We use time- and angle-resolved photoemission spectroscopy (trARPES) to show that this picture breaks down away from thermal equilibrium and on ultrafast time scales. We find that photo-doping of the graphene - buffer layer heterostructure increases the carrier concentration inside the Dirac cone. Supported by pump fluence and pump wavelength dependent measurements we attribute this transient charging to direct electronic transitions between the buffer layer and the graphene layer and subsequent relaxation of the non-equilibrium charge carrier distribution. [1] Phys. Rev. B 77, 155303 (2008)

# O 68: Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation IV

This focus session aims to discuss recent advances in the on-surface synthesis, manipulation, characterization, and understanding of complex molecular architectures on surfaces. The interest in surface-confined molecular nanostructures emerges from their prospective applications in nanoscale (opto-) electronics, spintronics, solar cells, energy storage devices, and other fields. The bottom-up fabrication of surface-supported nanostructures can be based on molecular self-assembly utilizing non-covalent intermolecular interactions, covalent on-surface synthesis, or the direct manipulation of molecules. Molecular self-assembly usually leads to highly ordered nanostructures, controlled by non-covalent interactions, adsorbate-substrate interactions, as well as thermodynamic and kinetic factors. On-surface synthesis by covalent coupling of reactive precursors adsorbed on metallic, semiconducting, or even insulating surfaces has emerged as a powerful method that has opened new possibilities in exploring new routes towards the synthesis of complex low-dimensional nanostructures with unprecedented material properties, often via novel chemical reactions not available in conventional organic chemistry. Finally, the direct manipulation of molecules with the tip of a scanning probe microscope allows for unprecedented chemical transformations or structural modifications, as envisioned by the pioneers of nanotechnology. This focus session is intended to provide a platform for addressing current trends in these closely linked fields from various perspectives in experiment and theory.

Organized by
Sabine Wenzel (University of Marburg) and Christian Wagner (Forschungszentrum Jülich)

Time: Wednesday 15:00–17:45 Location: H24

O 68.1 Wed 15:00 H24

**On-surface Synthesis of Aza-Coronoids** — •Tim Naumann[1], Zilin Ruan[1], Olaf Kleykamp[1], Alix Kaczmarek[2], Linus Pohl[2], Andreas Achazi[2], Eugen Sharikow[1], Doreen Mollenhauer[2,3,4], Jörg Sundermeyer[1], and J. Michael Gottfried[1] — [1]Philipps-Universität Marburg, Hans-Meerwein-Str. 4, 35032 Marburg, Germany — [2]Justus Liebig Universität Gießen, Heinrich-Buff-Ring 17, 35392 Gießen, Germany — [3]Helmholtz-Institut für Polymere in Energieanwendungen, Lessingstr. 12-14, 07743 Jena, Germany — [4]Institut für Technische Chemie und Umweltchemie, Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

The properties of nanographenes can be tailored by altering the topology, introducing defect sites like vacancies, or doping with heteroatoms. Coronoids represent a versatile sub-class of the nanographenes and can be regarded as benzenoids featuring a cavity. In-solution synthesis of extended coronoids has shown to be challenging due to their low solubility. To gain access to various aza-coronoids, we combined in-solution and on-surface techniques. By modification of the precursor's substituents, the edge termination of the coronoids is controlled. Besides planar armchair-edge and zigzag-edge terminated coronoids, a curved coronoid was synthesized. Nitrogen functionalization of the cavity allows for hosting a metal atom, giving rise to the formation of coronoid-metal complexes. The electronic and geometric properties of the nanostructures were investigated by low temperature scanning tunneling microscopy/spectroscopy (STM/STS) and non-contact atomic force microscopy (nc-AFM) and supported by DFT calculations.

O 68.2 Wed 15:15 H24

**Sequential on-surface synthesis of planar and curved fused anthracenyl-porphyrins** — •Miloš Baljozović[1], Joffrey Pijeat[2], Stéphane Campidelli[2], and Karl-Heinz Ernst[1,3,4] — [1]Empa, Dübendorf, Switzerland — [2]Université Paris-Saclay, CEA, Gif-sur-Yvette, France — [3]University of Zürich, Zürich, Switzerland — [4]The Czech Academy of Sciences, Prague, Czech Republic

On-surface synthesis has lately provided means for C-C bond formation that would otherwise hardly be accessible by conventional solution chemistry. Porphyrins are of particular interest in this regard, due to the ability to fine tune their physical and chemical properties via central metal incorporation or peripheral functionalization. Nevertheless, the formation of $\pi$-extended porphyrins bearing unsubstituted anthracenyl moieties was so far not achieved.

In this contribution we demonstrate temperature controlled (cyclo)dehydrogenation of bis- and tetra-anthracenyl Zn(II) porphyrins on a Au(111) substrate. Notably, on-surface dehydrogenation is not limited to the first dehydrogenation step involving fusion of anthracenyl units to the macrocycle. Sequential dehydrogenation with temperature elevation is leading to novel planar and curved porphyrin products beyond ones obtained by wet synthesis that could be identified in our combined STM, XPS and ToF-SIMS study.[1]

Support by Swiss National Science Foundation and University of Zürich Research Priority Program LightChEC is gratefully acknowledged.

[1] Baljozović, M. et al. J. Am. Chem. Soc. - just accepted.

O 68.3 Wed 15:30 H24

**On-surface synthesis of porphyrin-capped carbon nanocones** — Nemanja Kocic[1], Andreas Dörr[1], Moritz Villmow[1], Kevin Dhamo[2], Michael Ruppel[2], Norbert Jux[2], Bernd Meyer[2], and •Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

We demonstrate the surface-assisted transformation of porphyrin-based precursor molecules into bowl-shaped nanographenes through cyclization reactions on an Au(111) surface. The structures are visualized by scanning probe techniques with submolecular resolution, directly revealing intramolecular bonding and compared to density-functional theory calculations. Distinct configurations that suggest bowl-to-dome inversion are identified on the surface. Additionally, we report the accompanying metallation of the macrocycle with Au substrate adatoms. This combination of porphyrin and nanographene with a periphery solely consisting of six-membered all-carbon rings might serve as a seed for growing porphyrin-doped graphene sheets.

O 68.4 Wed 15:45 H24

**Relating Radical Delocalization, Charge Transfer and Magnetic Ground State in Open-Shell Molecules** — Tao Wang[1], Sergio Salaverria[2], Fernando Aguilar-Galindo[3], Javier Besteiro-Saez[4], Luis M. Mateo[4], Paula Angulo-Portugal[5], Jonathan Rodriguez-Fernandez[6], Dolores Perez[4], Martina Corso[1,5], Diego Peña[4], and •Dimas G. de Oteyza[1,2] — [1]Donostia International Physics Center, San Sebastián, Spain — [2]Nanomaterials and Nanotechnology Research Center (CINN), El Entrego, Spain — [3]Universidad Autónoma de Madrid, Madrid, Spain — [4]CiQUS, Santiago de Compostela, Spain — [5]Centro de Fisica de Materiales, San Sebastián, Spain — [6]University of Oviedo, Oviedo, Spain

At the same time as our capabilities to synthesize open-shell carbon-based materials are rapidly growing with the development of on-surface synthesis under vacuum conditions, the interest in pi-magnetism is rising due to its excellent prospects for potential applications. As a result, increasing efforts are being focused on the detailed understanding of open-shell carbon nanostructures and all the parameters that determine their spin densities and magnetic ground states. Here we present a facile route to synthesize different open-shell acene derivatives with closely related structures. A systematic comparison allows us to draw conclusions on the role of the functional groups, their number and distribution, as well as on the role of the radical state delocalization in relation with the presence or absence of charge transfer at interfaces, which consequently impacts the molecules pi-magnetism.

O 68.5 Wed 16:00 H24

**A route toward the on-surface synthesis of organic ferromagnetic quantum spin chains** — •Fabian Paschke[1], Ricardo Ortiz[2], Shantanu Mishra[1], Manuel Vilas-Varela[3], Florian Albrecht[1], Diego Peña[3], Manuel Melle-Franco[2], and Leo Gross[1] — [1]IBM Research Europe - Zurich, 8803 Rueschlikon, Switzerland — [2]CICECO - Instituto de Materiais de Aveiro, 3810-193 Aveiro, Portugal — [3]CiQUS and Department of Organic Chemistry, 15782 Santiago de Compostela, Spain

Engineering a sublattice imbalance is an intuitive way to induce high-spin ground states in bipartite polycyclic conjugated hydrocarbons. Such high-spin molecules can be employed as building blocks of quantum spin chains, which are outstanding platforms to study many-body physics and fundamental models in quantum magnetism [1].

In contrast to antiferromagnetism, demonstration of ferromagnetic coupling between polycyclic conjugated hydrocarbons has been scarce. Here, we demonstrate the on-surface synthesis of short ferromagnetic spin chains based on dibenzotriangulene, a polycyclic conjugated hydrocarbon with a triplet ground state. We achieve a direct majority-minority sublattice coupling between adjacent units, which leads to a global sublattice imbalance in the chains and therefore a ferromagnetic ground state with a strong intermolecular ferromagnetic exchange. By means of scanning probe measurements and quantum chemistry calculations, we confirm quintet and septet ground states in dimers and trimers, respectively.

[1] S. Mishra et al., Nature 598, 287 (2021).

O 68.6 Wed 16:15 H24

**Atomically Precise Control of Topological State Hybridization in Conjugated Polymers** — Alejandro Jiménez-Martín[1,2], Zdenka Sosnová[2], Diego Soler[2], Benjamin Mallada[1], Héctor González-Herrero[1], Shayan Edalatmanesh[1,2], Pavel Jelínek[1,2], and •Bruno de la Torre[1,3] — [1]Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute (CATRIN), Palacký University, 78371 Olomouc, Czech Republic — [2]Institute of Physics of the Czech Academy of Sciences, 16200 Prague, Czech Republic — [3]Nanomaterials and Nanotechnology Research Center (CINN), CSIC-UNIOVI-PA, 33940 El Entrego, Spain

Realization of topological quantum states in carbon nanostructures has recently emerged as a promising platform for hosting highly coherent and controllable quantum dot spin qubits. However, their adjustable manipulation remains elusive. Here, we report the atomically accurate control of the hybridization level of topologically protected quantum edge states emerging from topological interfaces in bottom-up-fabricated $\pi$-conjugated polymers. Our investigation employed a combination of low-temperature scanning tunneling microscopy and spectroscopy, along with high-resolution atomic force microscopy, to effectively modify the hybridization level of neighboring edge states by the selective dehydrogenation reaction of molecular units in a pentacene-based polymer and demonstrate their reversible character.

O 68.7 Wed 16:30 H24

**On-surface encapsulation of azafullerene radicals: towards 2D spin networks** — •Marion A. van Midden Mavrič[1], Bastien Anézo[1,2], Gregor Kladnik[3,4], Luca Schio[4], Gregor Bavdek[4,5], Yuri Tanuma[1,6], Ruben Canton-Vitoria[7], Ioanna K. Sideri[7], Nikos Tagmatarchis[7], Jannis Volkmann[8,9], Herman A. Wegner[8,9], Andrea Goldoni[10], Chris Ewels[2], Alberto Morgante[4,11], Luca Floreano[4], Erik Zupanič[1], Dean Cvetko[1,3,4], and Denis Arčon[1,3] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]IMN, Nantes University, France — [3]FMF, University of Ljubljana, Slovenia — [4]CNR-IOM, Trieste, Italy — [5]PF, University of Ljubljana, Slovenia — [6]CAREM, Hokkaido University, Sapporo, Japan — [7]T.P.C.I., Athens, Greece — [8]Center for Materials research, Giessen, Germany — [9]Justus Liebig University, Giessen, Germany — [10]Elettra Sincrotrone Trieste S.C.p.A., Italy — [11]Phys. dept., University of Trieste, Italy

While organic radicals on surfaces are a promising platform for realizing and controlling qubits, they are usually highly reactive. Here we present on-surface encapsulation of azafullerene $C_{59}N^\bullet$ into [10]cycloparaphenylene ([10]CPP) nanohoops on Au(111) as an efficient strategy to form supramolecular complexes with long-term spin protection. By vacuum depositing $C_{59}N^\bullet$ on a pre-deposited template layer of [10]CPP, extended networks of spin 1/2 radicals in a hexagonal lattice are formed. We find compelling evidence for electronic coupling between both molecular species, show that [10]CPP protects $C_{59}N^\bullet$ against dimerization and inhibits coupling to the Au(111) substrate.

O 68.8 Wed 16:45 H24

**Remote debromination on ultrathin insulating film** — •Tzu-Chao Hung[1], Lucía Gómez-Rodrigo[2], Lennart Moritz[1], Manuel Vilas-Varela[2], Leo Gross[3], Diego Peña[2], and Jascha Repp[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS) and Departamento de Química Orgánica, Universidade de Santiago de Compostela, Spain — [3]IBM Research Europe, Zurich, Switzerland

Open-shell carbon-based structures are widely studied in recent years not only owing to their potential applications in spintronics and as quantum devices, but they can also serve as a platform to investigate electron-correlation phenomena. One way to study open-shell molecules despite their large reactivity, is to create them from a suitable precursor in a scanning probe microscope (SPM) under ultra-high-vacuum and low-temperature conditions. Here, we demonstrate a particularly efficient debromination reaction resulting in an open-shell molecule by means of SPM manipulation on ultrathin NaCl film on Cu(111). The debromination even works remotely with the tip being up to ˜10 nm away from the molecule for both voltage polarities. Based on our observation, possible reaction mechanisms will be discussed.

**Invited Talk** O 68.9 Wed 17:00 H24

**On-Surface Synthesis of Porphyrins and BN-Substituted Carbon Scaffolds** — •Willi Auwärter — Technical University of Munich, Garching, Germany

On-surface synthesis protocols provide elegant routes to individual molecular complexes, oligomers, and other carbon-based nanomaterials on metal supports [1]. The resulting structural, physical, and chemical properties can be controlled by heteroatom-substitution. The talk will report on our activities employing thermally induced reactions on coinage metal surfaces, affording heteroatom-doped porphyrins and BN-substituted carbon scaffolds. Specifically, a route to peripherally O-doped porphyrins is addressed [2]. Furthermore, we will discuss the use of functionalized borazine precursors yielding covalent carbon networks with $(BN)_3$ motifs. These include random sheet-like BNC structures [3], which can be transferred to Si waver dices, and covalent organic frameworks (COFs) on Ag(111) and Au(111). The comprehensive characterization by scanning probe microscopy, complemented by theoretical modelling, reveals that COFs with distinct $(BN)_3$ densities, pore sizes, and electronic structures can be achieved. The findings open pathways to new O- and BN-substituted carbon-based nanoarchitectures on surfaces. [1] Grill, L.; Hecht S. Nat. Chem. 12, 115 (2020). [2] Deyerling, J. et al. Angew. Chem. Int. Ed., e202412978 (2024). [3] Tömekce et al., Chem. Eur. J., e202402492 (2024).

O 68.10 Wed 17:30 H24

**An electrically controlled molecular spin switch** — •Kwan Ho Au-Yeung[1], Wantong Huang[1], Paul Greule[1], Máté Stark[1], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], Roberto Robles[2], Nicolas Lorente[2,3], and Philip Willke[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), 20018 Donostia-San Sebastián, Spain — [3]Donostia International Physics Center, 20018 Donostia-San Sebastián, Spain

Precise control of spin states and spin-spin interactions in atomic-scale molecular complexes is key to developing multi-spin systems on surfaces for instance for applications in quantum technologies. This has been realized in a variety of systems, for instance in spin-crossover molecules. In this study, we explore the spin coupling and tunability of molecular dimer complexes on an insulating magnesium oxide film: When brought close to a single Fe adatom, a FePc molecule interacts with the Fe forming an interacting spin system. The calculated adsorption geometries by density functional theory (DFT) shed light on the two adsorption configurations of the two bistable states. The two states of the Fe-FePc complex can be successfully and reversibly switched using STM voltage pulses. Subsequently, by using scanning tunneling spectroscopy, we show that this is accompanied by an alteration of the total spin state and spin coupling in the complex. We further illustrate how the complex can be used to shift the resonance frequency of a nearby FePc in single spin resonance experiments, which demonstrates that this complex can function as a magnetic spin switch.

## O 69: Nanostructures at Surfaces II

Time: Wednesday 15:00–17:30 Location: H25

O 69.1 Wed 15:00 H25

**Thermally-activated molecular rotors organised by porous networks on Au(111)** — •Vishakya Jayalatharachchi[1], Roberto Robles[2], Milan Kivala[3], Nicolás Lorente[2,4], Meike Stöhr[1,5], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastián, Spain — [3]Institute of Organic Chemistry, University of Heidelberg, Germany — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain — [5]University of Applied Sciences of the Grisons, Switzerland

Gaining insights into the precise control of molecular rotation on surfaces is crucial for making progress in nanoscale device innovation. In this study, we investigate the thermally triggered rotational motion of bromine-functionalized decacyclene (Br-DC) molecules, which are confined within a host-guest network of 4,4,'4"-nitrilotribenzoic acid (H3NTB) on Au(111). With scanning tunneling microscopy (STM) experiments at variable temperatures, we could determine both the onset of molecular rotation (around 110 K) and the barrier for rotation. Importantly, the Br-DC molecules do not possess a predefined intrinsic rotation axis. Instead, the rotational motion is facilitated by the attractive interactions between the Br-DC guests and the H3NTB host network. Computational simulations support our findings and provide further insights into the energetics. Our strategy provides greater flexibility and versatility compared to traditional confinement approaches based on precise size matching of rotor and host networks.

O 69.2 Wed 15:15 H25

**Examination and Modification of Self-organized Nanostructures in the Ternary System Au/Co/Ge(001): Chain Growth and the Observation of a Zero-Bias Anomaly** — •Nico Kubetschek, Till-Jakob Stehling, Ulrike Kürpick, Marcel Schlesag, Johann Tonhäuser, and René Matzdorf — Institute of Physics, University of Kassel, Heinrich-Plett-Str. 40, Kassel D-34132, Germany

The twofold symmetric reconstruction of the Ge(001) surface provides a template for the self-organized formation of various transition metal nanostructures [1]. We employed scanning tunnelling microscopy (STM) and spectroscopy (STS) at 77 K and 5 K to examine the nucleation, chain growth, and subsequent modification of hexagonal cobalt nanostructures embedded in Ge(001) [2] through the introduction of gold-induced defects [3]. Moreover, the introduction of additional amounts of Au resulted in the formation of previously unobserved nanorods [4]. The electronic properties of these rods were examined by STS, which revealed a zero-bias anomaly (ZBA) in the tunneling spectra. The formation of nanorods with high aspect ratios was subjected to a systematic statistical investigation.

[1] J. Schäfer et al. 2009, New J. Phys. 11 125011, [2] H. J.W. Zandvliet et al. 2011, Surface Science 605,1129, [3] J. Tonhäuser et al. 2022 Phys. Rev. B 106, 115404, [4] M. Schlesag et al. 2024 Phys. Rev. B 110, 195412

O 69.3 Wed 15:30 H25

**Electrical Modulation of a Plasmonic Single Particle Resonance** — Luka Zurak[1], Christian Wolff[2], Jessica Meier[1], René Kullock[1], •Asger Mortensen[2], Bert Hecht[1], and Thorsten Feichtner[1] — [1]Nano-Optics and Biophotonics Group, Experimentelle Physik 5, Universität Würzburg, 97074 Würzburg, Germany — [2]POLIMA Center for Polariton-driven Light-Matter Interactions, University of Southern Denmark, DK-5230 Odense M, Denmark

Acitive modulation of plasmonic resonances is a promising route towards optical switches smaller way that than the diffraction limit. However, due to the difficulties to directly electrically connect a single resonator most experiments in this direction have been performed on large scales and/or in electrochemical environments – hampering interpretation and application.

Here, we demonstrate fast modulation of the plasmonic resonance of a single electrically connected gold nano-rod [1]. We employ a lock-in amplifier to measure the relative change of scattering signal $\Delta S/S_0$ in the spectral range from 500 to 900 nm, while driving our structure with up to 50 kHz in frequency and up to 40 V in voltage amplitude. Results are of the expected order of magnitude according to existing theories. We discuss some of the theories in detail, like classical surface currents or the introduction of Feibelman parameters to account for non-classical electron spill-out at metal surfaces.

[1] Zurak, L., et al. (2024). Modulation of surface response in a single plasmonic nanoresonator. Science Advances, 10(36), eadn5227.

O 69.4 Wed 15:45 H25

**On-surface induced fitting and mobility of conformationally flexible molecules inside nanometer-sized quantum confinements** — Aisha Ahsan[1,2], •Aaron Oechsle[2,1], Luiza Buimaga-Iarinca[3], Lutz H. Gade[4], and Thomas A. Jung[2,1] — [1]Department of Physics, University of Basel, 4056 Basel, Switzerland — [2]Laboratory for Micro and Nanotechnology, Paul Scherrer Institute, 5232 Villigen, Switzerland — [3]CETATEA, National Institute for Research and Development of Isotopic and Molecular Technologies, 400293 Cluj-Napoca, Romania — [4]Institute of Inorganic Chemistry, University of Heidelberg, 69120 Heidelberg, Germany

Host-guest architectures provide ideal systems to investigate site-specific physical and chemical effects. Condensation events in nanometer sized confinements are particularly interesting for the investigation of inter-molecular and molecule-surface interactions. They may be accompanied by conformational adjustments representing induced-fit packing patterns. Here, we report that the symmetry of small clusters of cycloalkane molecules, formed by condensation, their registry with the substrate, their structure as well as their adsorption height is characteristically modified by their packing in confinements. While cyclopentane and cycloheptane display cooperativity upon filling of the hosting pores, cyclooctane and to a lesser degree cyclohexane diffusively re-distribute to more favored adsorption sites. The site-specific modification of the interaction and behavior of adsorbates in confinements plays a crucial role in many applications of porous materials, e.g., as gas storage agents or catalysts and biocatalysts.

O 69.5 Wed 16:00 H25

**Areas of lower local contact potential difference in the wetting layer in the system Pb/Si(111)-(7x7)** — •Paul Philip Schmidt[1], Felix Hartmann[1], Ralf Metzler[1,2], Janet Anders[1,3], and Schmidt Hoffmann-Vogel[1] — [1]University of Potsdam, Institute of Physics and Astronomy, Germany — [2]Asia Pacific Center for Theoretical Physics, Pohang 37673, Republic of Korea — [3]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter EX4 4QL, UK

The description of the diffusion of Pb atoms on Si(111)-(7x7) is highly non-trivial. Previous studies show that although Pb grows in the Stranski-Krastanov mode, it exhibits explosive island growth and ultrafast mass transport [1,2]. The developing wetting layer plays a special role [3]. We have investigated this system using non-contact scanning force microscopy and Kelvin probe force microscopy. We have worked under ultrahigh vaccum conditions at variable temperatures between 120K and 300K. Our studies show inhomogeneities of the work function in the wetting layer. The areas with different work function seem to be related to the position of the islands and the step edges of the Si(111). We assume that the different work function values are caused by different Pb concentrations in the wetting layer, which are probably related to the preferred direction of growth of the islands, so that in certain areas Pb is extracted from the wetting layer with varying effectiveness. [1] M. Hupalo et. al. Phys. Rev. B, 23 (2007), [2] K. L. Man et al. Phys. Rev. Lett., 101 (2008), [3] M. T. Hershberger et al. Phys. Rev. Lett. 113 (2014)

O 69.6 Wed 16:15 H25

**Pyridyl-functionalized tripod molecules on Au(111): Inter-**

**play between hydrogen bonding and metal coordination** — •Sajjan Mohammad[1], Neeta Bisht[2], Anjana Kannan[1], Anne Brandmeier[2], Christian Neiss[2], Andreas Görling[2], Meike Stöhr[1,3], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, Chair of Theoretical Chemistry, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]University of Applied Sciences of the Grisons, Switzerland

Two-dimensional metal-organic coordination networks (MOCNs) offer rich opportunities for fabricating materials with potential applications in catalysis and molecular electronics. We investigated the self-assembly of pyridyl-functionalized triazine (T4PT) on Au(111) using low-temperature scanning tunneling microscopy (STM) complemented by density functional theory (DFT) calculations. T4PT forms a well-ordered, close-packed structure stabilized by hydrogen bonds upon adsorption at 300 K. Upon post-deposition annealing, the assemblies are additionally stabilized by metal-ligand bonding between the pyridyl ligands and native Au adatoms. Further post-deposition annealing to 473 K led to the breaking of the N-Au bonds, with the molecular assemblies transforming into a second close-packed hydrogen-bonded structure. Above 503 K, few covalently linked dimers formed, likely as a result of CH-bond activation. Our findings highlight the challenge of predicting and controlling 2D structure formation for porous MOCNs on metal surfaces due to competing interactions.

O 69.7 Wed 16:30 H25

**Active manipulation of interface electronic structures by two-dimensional metal-organic coordination on metallic substrates** — •Lu Lyu[1,2], Jonas Gödde[2], Martin Anstett[2], Martin Aeschlimann[2], and Benjamin Stadtmüller[1] — [1]Experimentalphysik II, Institute of Physics, Augsburg University, 86159 Augsburg, Germany — [2]Department of Physics, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Designing two-dimensional metal-organic coordination networks (2DMOCNs) on metallic substrates provides a unique approach for engineering interface electronic structures. To achieve this goal, we first investigate a protocol of pyridine-functionalized T4PT molecules with Co coordination (Co-T4PT) adsorbed on Au(111). In this system, the surface state electrons are bound to the Co metal centers, and charge transfer occurs between the Co and the substrate. By substituting the Co center with a Cu atom, the surface state electrons in the Cu-T4PT coordination exhibit weaker binding to the Cu centers and are partially confined within the pores surrounded by the molecular potentials. Additionally, replacing T4PT with cyano-functionalized DCA enhances the coordination between Co and DCA, resulting in altered charge transfer within the Co-DCA plane. Consequently, the orbital states of DCA undergo modifications in both energy and momentum space. Our study demonstrates that the manipulation of coordinated metals and functionalized molecules can actively tailor electronic structures at a 2DMOCN-metal interface.

O 69.8 Wed 16:45 H25

**Unveiling hybrid electronic bands in 2D metal-organic frameworks: insights from density functional theory and photoemission spectroscopy** — Dominik Brandstetter[1], Simone Mearini[2], Yan Yan Grisan Qiu[2], Daniel Baranowski[2], Andreas Windischbacher[1], Claus Michael Schneider[2,3], Vitaliy Feyer[2,3], and •Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]PGI-6, FZ-Jülich, Germany — [3]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

Two-dimensional metal-organic frameworks are atomically thin materials that combine properties of organic molecules with the characteristics of crystalline inorganic solids. The strong bonding between the organic linkers and transition metal centers may result in new electronic states with hybrid organic/inorganic character, from which two-dimensional, dispersing electronic bands emerge. However, until recently no experimental proof for such hybrid bands could be given and the requirements for efficient hybrid band formation remained unknown. Here, we combine density functional theory calculations with experimental angle-resolved photoemission spectroscopy to reveal the nature of the interaction between the transition metal atoms and the organic linker. On the example of the Ni-TCNQ network supported on Ag(100) and by employing photoemission orbital tomography, we observe how the molecular orbitals hybridize with the Ni d-states of appropriate symmetry. Our findings are not only based on electronic structure theory, but are also confirmed by the experimental photoemission fingerprints of the involved molecular orbitals.

O 69.9 Wed 17:00 H25

**Atomic size effects in 1D metal-coordination polymers on silver** — •Pengfei Zhao[1], Hongxiang Xu[1,3], Joachim Reichert[1], Anthoula C. Papageorgiou[1,2], and Johannes V. Barth[1] — [1]Technical University of Munich, Germany — [2]National and Kapodistrian University of Athens, Greece — [3]Peking University, China

Supramolecular coordination on solid surfaces provides a versatile approach to synthesize one-dimensional metal coordination polymers (1D-CPs), where the atomic size of metals plays a crucial role in determining the final structures and properties. Here, we systematically investigate 1H,1'H-2,2'-bibenzo[d]imidazole ($H_2$bbim) on silver substrates under ultra-high vacuum. Using scanning probe microscopy, we find that the shape of 1D-CPs can be steered by metal-coordination templating with different metal atom sizes. Specifically, $H_2$bbim molecules and cobalt atoms on Ag(100) allow the formation of micrometer-sized 1D-CPs with porphyrinoids formed by covalently fused $H_2$bbim dimers, which is distinct from its counterpart of holmium-coordinated chains of monomers. This suggests that size-tuned metal templating is a good strategy for tailoring the formation of 1D-CPs, demonstrating its potential for next-generation electronic devices.

O 69.10 Wed 17:15 H25

**An insight into the thermally activated organometallic-to-covalent transition in novel Graphdiyne Molecular Wires Frameworks** — •Alice Cartoceti[1], Simona Achilli[2], Paolo D'Agosta[1], Alessio Orbelli Biroli[3], Guido Fratesi[2], Valeria Russo[1], Andrea Li Bassi[1], and Carlo Spartaco Casari[1] — [1]Department of Energy, Politecnico di Milano, I-20133 Milano, Italy — [2]Department of Physics, Università degli Studi di Milano, I-20133 Milano, Italy — [3]Department of Chemistry, Università di Pavia, I-27100 Pavia, Italy

Graphdiynes (GDYs) are novel carbon allotropes with mixed sp-sp$^2$ hybridization, characterized by tunable optoelectronic properties. This study investigates the temperature-dependent atomic-scale structure and vibrational properties of 1,4-bBEB-based GDY molecular wires frameworks synthesized via Ullmann coupling on Au(100) and Au(111) surfaces. Scanning Tunnelling Microscopy revealed the transition from ordered frameworks of densely packed and oriented 1D organometallic wires (OMF) at room temperature, to progressively more disordered covalent frameworks (COF) at high temperatures. Density Functional Theory calculations and in situ Raman spectroscopy measurements tracked the OMF-to-COF transition, assigning specific Raman features to both phases. Raman spectroscopy also revealed that surface orientation influences the wires-gold interaction, resulting in a lower temperature for the OMF-to-COF transition on Au(100) than on Au(111).

## O 70: Poster Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules

Time: Wednesday 18:00–20:00 Location: P2

O 70.1 Wed 18:00 P2

**Nitrogen Doping of Cuprous Oxide Films: A Surface Science Perspective** — Mina Soltanmohammadi and •Niklas Nilius — Carl-von-Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany

Nitrogen doping of $Cu_2O$ films grown on Au(111) and Pt(111) supports was explored by a variety of surface-science techniques, including electron-diffraction, X-ray photoelectron-spectroscopy (XPS), scanning tunneling microscopy and photoluminescence spectroscopy (PL). The films were prepared by Cu vapor deposition and high-pressure oxidation at 50 mbar $O_2$. Nitrogen was inserted by adding $N_2$ to the reactive gas or via sputter doping. Only the latter resulted in a clear N1s signal in XPS, compatible with the insertion of N-atoms at O substitutional sites. The N-doping caused an overall degradation of the oxide lattice and suppressed the formation of the $(\sqrt{3}\times\sqrt{3})R30^\circ$ surface reconstruction observed on pristine $Cu_2O(111)$. Moreover, the oxide Fermi level shifted from the valence-band top into the band gap, indicative for a reduced p-type conductivity of the sample upon doping. The N-dopants featured low thermal stability and largely desorbed at 500 K, leaving behind a pronounced 850 nm PL peak due to O vacancy emission. Our findings indicate that the N-atoms initially occupy O substitutional sites but get removed easily at moderate temperature, casting doubts whether N-doping is a suitable pathway to improve the conductance and luminescence behavior of $Cu_2O$.

## O 71: Poster Plasmonics and Nanooptics: Fabrication, Characterization and Applications

Time: Wednesday 18:00–20:00 Location: P2

O 71.1 Wed 18:00 P2

**Large area writing of $In_3SbTe_2$ metasurfaces for polarization optics and complex orbital angular momentum beams** — •Maike Kreutz[1], Lukas Conrads[1], Andreas Mathwieser[2], Matthias Wuttig[1], Robert Schmitt[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen — [2]Fraunhofer IPT

Optical metasurfaces enable tailoring light-matter interaction for miniaturized optical elements with customized functionalities.The nonvolatile reversible switching of phase-change materials (PCMs) has been applied for tunable optical metasurfaces [1]. The plasmonic PCM $In_3SbTe_2$ (IST) switches from an amorphous dielectric to a crystalline metallic state. IST has been exploited for the direct laser writing of metallic nanoantennas in a dielectric surrounding [2] and for geometric phase metasurfaces [3] including orbital angular momentum (OAM) beams with single singularities. Here, we investigate optical metasurfaces fabricated with the Nanoscribe Photonic Professional GT to shape OAM beams with multiple singularities. We show preliminary results regarding the optical programming of these OAM beams for possible applications in optical communications [4]. Additionally, metasurface polarization optics are explored, enabling plasmonic quarter-wave plates with large bandwidths in the infrared range. This work paves the way towards creating tailored reconfigurable metaoptics for the infrared without cumbersome fabrication techniques. [1] Wuttig et al., Nat. Photon. 11, 465 (2017), [2] Heßler et al., Nat. Commun. 12, 924 (2021), [3] Conrads et al. arXiv:2408.05044 (2024), [4] Shen, Y. et al. Light. Sci. Appl. 8, 90 (2019)

O 71.2 Wed 18:00 P2

**Investigation of the plasmonic phase-change material $In_3SbTe_2$ in the near-infrared range** — •Hristiyana Kyoseva, Lukas Conrads, Rebecca Rahmel, Gero von Plessen, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

Phase-change materials (PCMs) provide a suitable platform for active nanophotonics and reconfigurable metasurfaces by enabling reversible switching between two phases with contrasting optical properties [1]. $In_3SbTe_2$ (IST) is a novel plasmonic PCM which can be switched between an amorphous (dielectric) and a crystalline phase (metallic in the whole infrared (IR) spectrum) with precise laser pulses [2]. The direct writing of micrometer-sized structures into a thin IST film with resonances in the mid-IR (above $5\,\mu m$) has been extensively demonstrated [3]; however, smaller structures have not been explored yet due to their challenging fabrication process. Here, we examine the smallest achievable sizes of structures written in IST by spatially overlapping crystallization and amorphization pulses. We investigate the resonances of sub-micrometer rod antenna arrays as they shift to shorter wavelengths (below $4\,\mu m$) with decreasing size. We also aim to identify its lower limit set by the refractive index of the surrounding media. Our work paves the way towards sophisticated antenna structures with resonances at shorter wavelengths, broadening the applications of IST as a versatile platform for active nanophotonics. [1] Wuttig et al. *Nat. Photon.* **11**, 465 (2017) [2] Heßler et al., *Nat. Com.* **12**, 924 (2021) [3] Heßler, Conrads et al., ACS Photon. **9**, 5 (2022).

O 71.3 Wed 18:00 P2

**Laser pulse front tilt effects in the observation of SPPs using photoemission electron microscopy** — •Hanno Christiansen[1], Tobias Eul[1], and Michael Bauer[2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

In recent years, PEEM has become an established technique for the investigation of surface plasmon polaritons (SPP). This technique allows, for example, the study of the propagation dynamics of these collective surface excitations with femtosecond resolution or the measurement of their dispersion relations with high spatial resolution. The characteristic signal measured in PEEM results from the coherent superposition of the exciting laser field and the emitted SPP. Based on simulations and experimental data we show in this contribution that the plasmonic PEEM signal is very sensitive to the pulse front tilt of the exciting laser pulse and thus represents a sensor for this often overlooked laser parameter.

O 71.4 Wed 18:00 P2

**Surface plasmon polariton neuronal cell** — •Emily Kruel[1], Christopher Weiss[1], Tobias Eul[2], Mario Pfeiffer[1], Benjamin Stadtmüller[3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern-Landau, Germany — [2]Institute of Experimental and Applied Physics, University of Kiel, Germany — [3]Institute of Physics, University of Augsburg, Germany

Today, the classical electronic computer architecture is one of the limiting factors for fast and energy-efficient data processing. This has triggered the search for alternative hardware architectures to overcome these limitations. For instance, neuromorphic photonics has emerged as a novel research field for new classes of information processing devices that incorporate photonically integrated neural networks [1].

The hybrid nature of surface plasmon polaritons (SPPs) offers a concept for integrating neuromorphic photonics by combining photonic advantages such as high bandwidth and speed with strong electronic interactions. Here, we present an experimental approach to constructing essential components of an artificial neuron based on SPP interactions. We optimized the dimensions of individual components through a combination of finite-difference time-domain (FDTD) simulations and iterative experimental adjustments. The resulting plasmonic responses are imaged using a photoemission electron microscope (PEEM).

[1] Shastri, B.J., Tait, A.N., Ferreira de Lima, T. et al., Nat. Photonics 15, 102-114 (2021)

O 71.5 Wed 18:00 P2

**Investigating Gel Electrolyte Compositions for Enhanced Switching Speed in PEDOT:PSS Electrochromic Devices and Switchable Metasurfaces** — •Hoorieh Fallah[1], Dominik Ludescher[1], Jonas Herbig[1], Mario Hentschel[1], Andy Steinmann[1], Klaus Dirnberger[2], Junqi Lu[2], Semi Kim[2], Aldilene Santos Franca[2], Sabine Ludwigs[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of

Stuttgart — [2]Institute of Polymer Chemistry, University of Stuttgart

Switchable metasurfaces using the conductive polymer PEDOT:PSS have gained substantial interest over the last years. PEDOT:PSS can be switched from metallic to dielectric state for wavelengths $> 1.3$ $\mu$m using electrochemistry, with CMOS compatible voltages between -1V to +1V. Here, we report on the preparation and characterization of gel electrolytes for PEDOT switching with varying ratios based on polyethylene oxide (PEO), polyvinyl alcohol polymers (PVA), acetonitrile, and lithium perchlorate ($LiClO_4$). Our gel electrolytes are integrated with PEDOT:PSS, coated onto ITO substrates to evaluate their performance in electrochromic switching applications. By applying alternating voltage and laser light, we analyze the dynamic switching speed of the PEDOT layer as it transitions from a conductive to an insulating state. Our approach explores how PEO- and PVA-based electrolytes impact high-frequency, low-voltage switching in PEDOT:PSS systems. We have achieved switching rates up to 100 Hz. The results aim to enhance our understanding of the influence of the electrolyte composition on switching behavior.

## O 72: Poster Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy

Time: Wednesday 18:00–20:00 Location: P2

O 72.1 Wed 18:00 P2

**Implementation of a fiber-based cathodoluminescence detector system for a scanning electron microscope** — •Filip Majstorovic[1], Paul H. Bittorf[1], and Nahid Talebi[1,2] — [1]Institute for Experimental and Applied Physics, Kiel University, Leibnizstraße 19, D-24118 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, Christian-Albrechts-Platz 4, D-24118 Kiel, Germany

Cathodoluminescence (CL) is the light emitted from materials irradiated with the electron beam, within the infrared to ultraviolet spectral range. CL recently has gained a major interest in analyzing quantum materials and emitters, thanks to its high spatial and temporal resolutions. In our study, inside a scanning electron microscope (SEM) high energy and broad bandwidth electron beams are generated. The CL emission is then collected with a detector, consisting of a multimode fiber attached to piezo stages, which allows for nanometer precision movement of the fiber near the sample. We present the variety of possible measurements such a system allows. One component of this is obtaining the spectrum of the emitted light, that for example enables the investigation of plasmonic resonances. Further this detector system provides a way to measure the emission profile by scanning the fiber three-dimensionally along the sample. Such emission profiles give information about the processes responsible for this radiation and show if coherent or incoherent CL are more dominant. Moreover, higher-order correlations unravel a superbunching effect in CL generated from semiconducting samples.

O 72.2 Wed 18:00 P2

**Comprehensive Probing of Electron and Phonon Systems by Raman Scattering** — •Jan Kutschera[1], Marc Herzog[1], Wouter Koopman[1], Felix Stete[1], and Matias Bargheer[1,2] — [1]Institut für Physik & Astronomie, Universität Potsdam, Potsdam, Deutschland — [2]Helmholtz Zentrum Berlin, Berlin, Deutschland

Inelastic processes in light-matter interactions are crucial for understanding energy transport within solid-state materials, where energy is distributed between electron and phonon systems. Investigating these interactions provides deeper insights into fundamental processes relevant to plasmonics, optoelectronics, and optoacoustics. However, knowledge about the energy transfer dynamics within each system is also essential for a complete picture. By extending Raman spectroscopy to ultrashort timescales, we aim at analyzing the transient population dynamics of phonon modes and the interplay of different electronic bands to ultimately establish ultrafast Raman Spectroscopy which directly probes electron-electron, electron-phonon, and phonon-phonon interactions. Here, we present an intraband emission of the conduction band electrons in gold nanoparticles, which is excited by interband absorption and appears as a continuous background in static Raman experiments. Pump-probe experiments can help further examine the origin of this emission and the interaction of different electronic subsystems. Moreover, we investigate the phonon modes of HfN and other materials as potential candidates for the catalysis of light-driven reactions.

O 72.3 Wed 18:00 P2

**Adiabatic focusing of propagating Surface plasmon polaritons at gold nanotriangles** — •Gregor Stockmann, Felix Stete, and Matias Bargheer — Institut für Physik und Astronomie, Universität Potsdam, Deutschland

Surface plasmon polaritons (SPPs) are the collective oscillations of surface-near charges at a dielectric-metallic interface. Due to the Coulomb force, these oscillations can propagate along the surface. This effect can be utilized to spatially separate the laser excitation and a chemical reaction site. In this work, we use gold nano-triangles, to focus SPPs from a $\mu m$-sized excitation spot to the tip at the nanometer scale. We investigate the influence of different parameters on the propagation behavior of SPPs. Key parameters are the particle dimensions, excitation wavelength and the light polarisation.

O 72.4 Wed 18:00 P2

**Plasmon assisted catalysis of Ferricyanide by Gold-Nanoparticles with different sizes and light intensities.** — •Kyra Peikert, Wouter Koopman, and Matias Bargheer — Institut für Astronomie und Physik Universität Potsdam, Potsdam, Deutschland

In recent years plasmonic catalysis emerged as promising new field in photocatalysis. However, to improve its efficiency, a better understanding of its governing principles is required. In this study we investigate the reaction kinetics of the light driven reduction of ferricyanide catalyzed by gold nanoparticles of different sizes. To refill the holes generated by electron transfer to ferricyanide the hole scavenger Ethanol (EtOH) is added to the solution. We compare this situation to reactions in a purely aqueous solution. The kinetics under different light intensities including dark conditions help to understand the mechanisms. The results show indications of a charging effect of the particles due to the presence of the hole scavenger, which speeds up the reaction rate.

O 72.5 Wed 18:00 P2

**Single particle sample with gold nanorods for micro-spectroscopy** — •Alexandra Faber — Institut für Physik und Astronomie, Universität Potsdam, Deutschland

Nobel metal nanostructures show great potential for photocatalytical applications due to their broadband plasmonic absorption across the visible spectrum. Chemical reactions taking place at surfaces can be accelerated by several effects, including charge transfer and local heating. As one important factor, the accumulation of charges on the particle during a reaction process, is expected to have a large influence on the charge transfer process. In order to better understand the effects of photocharging of gold nanorods (GNR), possible electron transfer between individual GNRs and the substrate, single nanoparticles are studied by optical micro-spectroscopy. The samples are investigated by dark-field as well as scanning electron microscopy and must therefore fulfill different requirements. This includes that the sample must provide the necessary criteria such as conductivity and light transmission in order to be observed with both microscopy methods. At the same time, it should be possible to rediscover individual GNRs and the distance between the particles has to be large enough to allow spectroscopy of individual GNRs. We show the development and improvement of the sample preparation procedure as well as first recorded dark-field scattering spectra and fluorescence spectra of single GNRs.

O 72.6 Wed 18:00 P2

**Size effects on the plasmon resonance in silver cluster anions studied by energy-resolved photoemission** — •Norman Iwe[1], Klara Raspe[1], Franklin Martinez[1], Lutz Schweikhard[2], Karl-Heinz Meiwes-Broer[1,3], and Josef Tiggesbäumker[1,3] — [1]Institute of Physics, University of Rostock, Germany — [2]Institute of Physics, University of Greifswald, Germany — [3]Department of Life, Light and Matter, University of Rostock, Germany

Numerous applications ranging from efficient solar cells to cancer treatment profit from the interaction between nanoparticles and light. In the case of metal clusters, one often takes advantage of collective resonances of the valence electrons, which lead to a strong increase of the cross section at a certain wavelength. Previous studies already showed, that the resonance energy can be tuned via size and charge state of the nanoparticles. However, systematic measurements to explore the development of the plasmonic resonance in free metal clusters so far concentrate on small sizes.

We conduct photoelectron spectroscopy on anionic silver clusters $\mathrm{Ag}_N^-$ in a size range $N = 7 - 300$. By extracting photodetachment cross sections, we gain insights into the collective resonances. At $N = 55$, we observe a transition from a blueshift to a general redshift of the plasmon energies with decreasing cluster size. However, the resonance energies for sizes below $\mathrm{N} = 55$ are oscillating whereby the maxima are found at known electronic shell closures. On top, a splitting of the resonance is observed at a few smaller cluster sizes, hinting on a deformation of the particle.

O 72.7 Wed 18:00 P2

**Anisotropic photoelectron emission from individual Ag nanoparticles on silicon** — •Waqas Pervez[1,2], Kevin Oldenburg[1,2], Sylvia Speller[1,2], and Ingo Barke[1,2] — [1]Institute of Physics, University of Rostock, Germany — [2]Department of Life, Light & Matter, University of Rostock, Germany

Laser excitation of localised plasmons in nanoparticles can give rise to a vastly enhanced photoemission yield [1, 2]. Here we study detailed characteristics of the photoelectron emission process of size-selected nanoparticles with diameters around 10 nm, deposited from the gas phase onto silicon. To this end we employ femtosecond laser excitation with wavelengths around 800 nm and 400 nm, respectively, in a photoemission electron microscope (PEEM). The spatially resolved electron yield is investigated as a function of laser wavelength and polarisation. Furthermore, we report on photoelectron emission from individual, supported nanoparticles in reciprocal space. Upon resonant plasmon excitation we observe anisotropic electron yield that depends on the laser polarisation. The observed photon order, ranging from 2PPE to 5PPE, and the underlying excitation and emission mechanisms are discussed in view of the local near field distribution and the effect of the substrate.

[1] M. Rohmer et al., Phys. Stat. Solidi B 247, 1132 (2010)
[2] K. Oldenburg et al., J. Phys. Chem. C 123, 1379 (2019)

O 72.8 Wed 18:00 P2

**Near-field Fano spectroscopy of MaPbI3 nanoparticles** — Jinxin Zhan[1], Tom Jehle[1], Sven Stephan[1], •Sam Nochowitz[1], Ekaterina Tiguntseva[2], Sergey Makarov[2], Juanmei Duan[1], Petra Gross[1], and Christoph Lienau[1] — [1]Universität Oldenburg, D-26129, Germany — [2]St. Petersburg, Russia

Semiconducting halide perovskite nanoparticles support Mie-type resonances that confine light on the nanoscale in localized modes with well-defined spatial field profiles yet unknown near-field dynamics. We introduce an interferometric scattering-type near-field microscopy technique [1] to probe the local electric field dynamics at the surface of a single MAPbI3 nanoparticle [2]. The amplitude and phase of the coherent light scattering from such modes are probed in a broad spectral range and with high spatial resolution. In the spectral domain, we uncover a Fano resonance with a $2\pi$ phase jump. In the near-field dynamics, this Fano resonance gives rise to a destructive interference dip after a few femtoseconds. Mie theory suggests that the interference between electric quadrupole and magnetic dipole modes of the particle, with spectra affected by resonant interband absorption of MAPbI3, lies at the origin of this effect [3]. Our results open up a new approach for probing local near-field dynamics of single nanoparticles. [1] Zhan, J., et al. Advanced Photonics 2020, 2 (04) [2] J. Zhan et al., Nano Lett. 2024 [3] Tiguntseva, E. Y., et al. Nano Lett. 2018, 18 (2), 1185-1190.

O 72.9 Wed 18:00 P2

**Energy and momentum distribution of surface plasmon-induced hot carriers** — •Ellen Brennfleck[1], Christopher Weiss[1], Jannis Lessmeister[1], Tobias Eul[2], Benjamin Stadtmüller[3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern-Landau, Germany — [2]Institute of Experimental and Applied Physics, University of Kiel, Germany — [3]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 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 72.10 Wed 18:00 P2

**Self-organized plasmonic particles configurations in front of mirror** — •Aleksei Overchenko and Frank Cichos — Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig

Plasmonic particles and their field enhancement properties found wide applications in various fields. For example, they are used in Surface-Enhanced Raman Spectroscopy (SERS), plasmon-enhanced fluorescence, Photothermal Therapy and energy conversion. Field enhancement can be achieved by bringing two spheres into close proximity, placing a sphere on a mirror, fabricating bowtie antennas, or designing hybrid structures like particle-dielectric-mirror systems. In most cases, surface functionalization often requires complicated modification methods such as lithography and chemical binding, e.g., of DNA origami which leads to complicated and non-reconfigurable systems. Here, we deliberately manipulate induvial as well as multiple gold particles in front of a gold mirror by local laser-induced temperature fields generating thermo-osmotic flow. Multiple particle trapping is performed by focused laser that can divide in multiple independent beams via AOD. We characterize the resulting single, dimeric and higher order clusters, their plasmonic coupling and the coupling of the particles to a thin gold film by scattering spectroscopy. The distance between the film and particles is around 10 nm due to the second minimum of the DLVO-theory. Enhancement is described by sensing of biomolecules. The system is reconfigurable as no binding is required and analytes may be bound to the film to enable spatially resolved SERS.

O 72.11 Wed 18:00 P2

**Optical resonance tuning of micro- and nanoparticles with phase change materials in the near-infrared and visible range** — •Rebecca Rahmel, Hristiyana Kyoseva, Jonathan Müller, Lukas Conrads, Thomas Taubner, and Gero von Plessen — I. Institute of Physics (IA), RWTH Aachen University

Micro- and nanoparticles with scattering and absorption resonances promise interesting optical behaviour. These resonances are highly sensitive to the particle size, shape, and configuration, as well as the dielectric properties of both particle and surrounding medium [1]. Phase-change materials (PCMs) show high optical contrast when switched between their amorphous and crystalline phases [2], facilitating antenna resonance tuning based on a change in refractive index [3]. The novel plasmonic PCM $\mathrm{In_3SbTe_2}$ (IST) can be locally optically switched between the dielectric amorphous and the metallic (in the infrared) crystalline phase, enabling a sign change in permittivity [4]. While antenna resonance tuning with PCMs has been studied extensively, locally addressing PCMs below single particles has not been demonstrated yet. Here, we investigate the optical response of single polystyrene micro- and gold nanoparticles placed on thin films of IST and other PCMs and locally switch the PCMs to tune the particle resonances. Our work paves the way towards mode selection of nanoparticles beneficial for tuning of emitters and sensing applications.

[1] Dahmen et al. *Aust. J. Chem.* **60**, 447-456 (2007) [2] Wuttig et al. *Nature Photon* **11**, 465-476 (2017) [3] Michel et al. *Adv. Mater.* **31**, 1901033 (2019) [4] Heßler et al. *Nat. Com.* **12**, 924 (2021)

O 72.12 Wed 18:00 P2

**Analytical Theory of the Optical Inter- and Intraband Response in Noble Metals** — •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 metal nanostructures can be attributed to the interplay of electronic intra- and interband processes described by coupled Boltzmann-Bloch equations. In this set of coupled equations, the specific properties of the noble metal are addressed by an anisotropic electronic dispersion relation expanded in the vicinities of the X and L high symmetry points.

In order to address the dephasing of the inter- and intraband polarizations we consider near equilibrium electron-phonon scattering rates in random phase approximation to estimate relaxation timescales. Our approach allows to connect spectroscopic signatures directly to microscopic processes, not possible with simple Drude-Lorentz models.

O 72.13 Wed 18:00 P2

**Kinetics of hydrogen molecules on Ag(111) by tip-enhanced Raman spectroscopy** — Shuyi Liu[1,2], Jun Yoshinobu[3], Martin Wolf[1], Takashi Kumagai[4], and •Akitoshi Shiotari[1] — [1]Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]Huazhong University of Science and Technology, Wuhan, China — [3]University of Tokyo, Kashiwa, Japan — [4]Institute for Molecular Science, Okazaki, Japan

Surface diffusion is the first step for adsorbates to undergo characteristic chemical and physical phenomena such as self-assembly, catalytic reactions, and low-dimensional molecular transport. However, the characterization of highly diffusive molecules, such as physisorbed molecules, has been challenging even with scanning tunneling microscopy and its related techniques. In this study, we use tip-enhanced Raman spectroscopy (TERS) to sensitively detect hydrogen molecules physisorbed on Ag(111) at low temperatures around 10 K. Strong Raman peaks were observed only when the diffusive molecule entered the plasmonic tip-sample junction, while the peaks decayed by thermal desorption at higher temperatures. By monitoring the peak intensities and investigating its temperature dependence, we successfully analyzed the kinetics of hydrogen molecules on the surface. This demonstrates that TERS is useful for evaluating the dynamics of diffusive molecules.

## O 73: Poster Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules

Time: Wednesday 18:00–20:00 Location: P2

O 73.1 Wed 18:00 P2

**In-situ tritium contamination and decontamination of fusion-relevant materials** — •Elizabeth Paine[1], Dominic Batzler[2], James Braun[2], Robin Grössle[2], Philipp Haag[2], Marco Röllig[2], Marie-Christine Schäfer[2], Marius Schaufelberger[2], and Kerstin Trost[2] — [1]Eindhoven University of Technology, The Netherlands — [2]Tritium Laboratory Karlsruhe, Karlsruhe Institute of Technology, Germany

Nuclear fusion could offer a solution to the growing global demand for clean, sustainable and abundant energy. The deuterium-tritium fusion reaction offers a high energy yield and feasibility at achievable temperatures. However, the scarcity and radioactive nature of tritium pose significant challenges for its handling in fusion reactors. Tritium adsorption onto surfaces leads to challenges in licensing, process control and maintenance. Ozone is a known decontaminant and may provide a viable solution for the decontamination of these tritiated surfaces. Due to its strong oxidising nature, ozone reacts with the adsorbed tritium, which can then be evacuated. This study aims to investigate tritium accumulation and decontamination on the fusion-relevant materials: beryllium, EUROFER97 and tungsten. These are selected for their critical roles in reactor components and tritium-processing systems. The findings will provide insights into the behaviour of tritium in these materials and assess the potential of ozone-based decontamination techniques compared to established methods. This contributes to the development of effective strategies for tritium handling, decontamination and inventory management in future fusion reactors.

O 73.2 Wed 18:00 P2

**Role of the surface for adsorbate motors** — •Bensu Günay Ramovic[1], Grant Simpson[1], Mats Persson[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, 8010 Graz, Austria — [2]Department of Chemistry, University of Liverpool, Liverpool L69 3BX, United Kingdom

Molecular motors have the ability to perform uni-directional rotation or translation. In addition to such motors in nature, for instance kinesin, artificial molecular motors have seen great developments in the last decades. They have been studied intensely in solutions by averaging methods, but these cannot resolve individual motors. We have studied molecular motors on metal surfaces by scanning tunneling microscopy under ultrahigh vacuum and cryogenic temperatures, allowing us to track the motion of single molecules. Metallic surfaces generally play an important role for physical/chemical processes in molecular adsorbates. Here, we investigate adsorbate motors [1] on different metal surfaces in order to elucidate the role of the substrate for the molecular motion. It turns out that even rather small differences - maintaining the same surface symmetry, but changing the elemental composition - strongly affects the molecular configuration and motion.

[1] Simpson, G. J., Persson, M., & Grill, L. (2023). Adsorbate motors for unidirectional translation and transport. Nature, 621(7977), 82-86.

O 73.3 Wed 18:00 P2

**Poisoning resistance of GaPt SCALMS model systems** — •Christoph Wichmann[1,2], Michael Moritz[2], Haiko Wittkämper[2], Tzung-En Hsieh[3], Johannes Frisch[3], Macus Bär[2,3,4], Hans-Peter Steinrück[2], and Christian Papp[1] — [1]FU Berlin, Germany — [2]FAU Erlangen, Germany — [3]Helmholtz-Zentrum Berlin, Germany — [4]Helmholtz Institute Erlangen-Nürnberg Germany

Supported catalytically active liquid metal solutions (SCALMS) are a novel concept, where low amounts of a catalytically active transition metal is dissolved in another low melting metal, which acts as a matrix. The highly dynamic surface provides an interesting system offering high activity and remarkable stabilities for dehydrogenation reactions. For industrial applications, different challenges have to be met. One of them is the presence of catalytic poisons in the catalytic feed such as sulfur compounds. Therefore, a model system of a macroscopic GaPt droplet with a low Pt content (1 at.%) and nanoscopic GaPt particles were investigated during the exposure to thiophene as catalyst poison using X-ray photoelectron spectroscopy (XPS) under ultra-high vacuum and near-ambient pressure (0.1-0.2 mbar) conditions. The formation of Ga-sulfides at the surface of the catalyst is observed, leading to an accumulation of Pt in / under this layer. For higher temperatures (>650 K), the dissolution of the formed Ga-sulfides into the liquid metallic Ga-matrix is observed. In all cases, no Pt-sulfide was formed, indicating a resistance of the active Pt sites towards sulfur poisoning of SCALMS.

O 73.4 Wed 18:00 P2

**An XPS and molecular beam study of olefin adsorption on ultrathin ionic liquid films on Pt(111)** — •Laura Ulm, Cynthia C. Fernández, Leonhard Winter, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg

Solid catalysts with ionic liquid layer (SCILL) promise improvements for a wide range of applications, e.g. an enhanced selectivity of the 1,3-butadiene hydrogenation to 1-butene by coating a heterogeneous catalyst with thin ionic liquid (IL) films. We studied hydrocarbon adsorption as central step of this reaction by X-ray photoelectron spectroscopy combined with a supersonic molecular beam. Ultrathin films of three different ionic liquids with thicknesses below 1 nm were deposited onto a Pt(111) crystal in UHV by physical vapor deposition and characterized with XPS. These films were exposed to 1,3-butadiene or 1-butene from a supersonic molecular beam at 180 K. The coverage-dependent sticking coefficients of the two olefins were measured using the King-and-Wells method. With increasing IL pre-coverage, the total amounts of adsorbed olefins decreased until further adsorption was completely suppressed by the IL layer. The minimum IL coverage needed for complete suppression of adsorption and the differences between the ionic liquids will be discussed in the context of IL-induced selective 1,3-butadiene hydrogenation.

Supported by the DFG through SFB 1452 (Project ID: 431791331).

O 73.5 Wed 18:00 P2

**N heteroatom effects in large aromatic physisorbed adsor-**

**bates on metal surfaces: azabenzopyrene on Cu(111)** — •Henry Thake[1], Matthew Stoodley[1,2], David A. Duncan[2,3], and Reinhard J. Maurer[1] — [1]University of Warwick, UK — [2]Diamond Light Source, UK — [3]University of Nottingham, UK

Conjugated molecules at metal surfaces are bound by a subtle balance of short- and long-range interactions including charge transfer and dispersion interactions. As such, they represent a challenging opportunity to improve approximations to density functional theory (DFT) where accurate structural and spectroscopic benchmark measurements exist. Accurate structural predictions of the large aromatic molecules naphthalene and pyrene have shown weak adsorption in a flat geometry on Cu(111). Here, we present a combined computational and experimental study of a closely-related molecule featuring a single nitrogen heteroatom - azabenzopyrene on Cu(111). Based on DFT calculations, x-ray standing wave (XSW) structural characterisation, x-ray photoelectron (XPS) and near-edge adsorption fine structure (NEXAFS) spectroscopy simulations, we study the effect of the heteroatom on the adsorption of the conjugated molecule. We develop a structural model consistent with XSW structure determination and simulate XPS and NEXAFS signatures of the sole nitrogen species in the molecule. Nitrogen 1s XPS and K-edge NEXAFS spectra present multiple co-existing chemical environments for the nitrogen species, for which we present a model hypothesis.

O 73.6 Wed 18:00 P2

**Surface Charge Modification of Silver Substrates for Enhanced SERS Selectivity** — •Georgiana Ion, Stefania Dana Iancu, and Nicolae Leopold — Faculty of Physics, Babes-Bolyai University, 400084, Cluj-Napoca, Romania

Surface-enhanced Raman spectroscopy (SERS) uses the plasmonic properties of metallic nanoparticles for sensitive detection in complex matrices. A key challenge is controlling the detection of specific species. This study developed solid-state SERS substrates with optimized surface properties for selective detection of anionic and cationic analytes.

Citrate-capped silver nanoparticles (cit-AgNPs) were synthesized via the Lee-Meisel method, while hydroxylamine-reduced silver nanoparticles (hya-AgNPs) followed the Leopold-Lendl method. Concentrated nanoparticles were dried into 2 $\mu$L droplets on cover glass to create solid substrates. Raman spectra were obtained by immersing the substrates in 2 mL analyte solutions (Nile Blue, Crystal Violet, fumaric acid) using a 532 nm laser.

We found that adding $Ca(NO_3)_2$ only impacts selectivity when added to the colloidal form before drying, making it crucial for developing both substrate types. This optimized cit-AgNPs for anionic detection, while hya-AgNPs, covered with $Cl^-$ ions, selectively detected cationic analytes. Cationic detection can also occur on cit-AgNPs by adding NaCl to the solution. This work highlights how surface modifications enhance SERS substrate selectivity and provide a pathway for tailored systems for specific analyte detection in complex environments.

O 73.7 Wed 18:00 P2

**Water adsorption on Bi(111) surfaces calculated from first principles** — •Yingjie Xie, Adriana Bocchini, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Deutschland

Bismuth is a semimetal with unique electronic properties, including a strong spin-orbit coupling. Water adsorption on bismuth surfaces is interesting from both a scientific and technological point of view, since the material has numerous electrode applications ranging from analytical chemistry, environmental monitoring, and energy storage to seawater desalination. Surprisingly, relatively little and partially contradiction information is available on the interaction between Bi and water [1,2]. In the present contribution, density-functional theory is used to calculate the adsorption of single water molecules, water clusters and water thin films on Bi(111). We analyze in detail the molecule-molecule and molecule-substrate interaction and provide information on the diffusion characteristics. The calculations are discussed in the context of previous theory and experimental data.

[1] V. Ivanistsev, *et al.*, E. Lust, Surf. Sci. **609**, 91 (2013).

[2] W. Oh *et al.*, J. Phys. Chem. C, **122**, 23084 (2018).

O 73.8 Wed 18:00 P2

**Investigation of $Na^+$ ion solvation on the Cu(111) surface by STM** — •Anna Shugai and Karina Morgenstern — Physical Chemistry I, Ruhr-Universität Bochum, Bochum, 44801, Germany

Sodium-ion ($Na^+$) batteries offer great potential as an energy storage, making them an attractive alternative to the lithium-ion batteries. However, the practical realization is currently restricted due to the instability of the electrode-electrolyte interface. To reveal the reasons for it, we need to understand the underlying mechanisms that govern the process of $Na^+$ ion on-surface solvation. In this project, we use low-temperature scanning tunneling microscopy (STM) to get the locally resolved structure of $D_2O$-solvated $Na^+$ ions that are supported on the Cu(111) surface. First, the small $D_2O$ clusters, containing 10 to 20 molecules, were prepared on the Cu(111) surface. We compare them to the $D_2O$ clusters deposited on the $Na^+$-pre-covered Cu(111) surface. The results show that there is strong interaction between the $Na^+$ ion and the $D_2O$ solvent molecules. Accordingly, the solvation behaviour of $Na^+$ is more similar to that exhibited by the $Li^+$ ion, than to that of the $Cs^+$ ion.

O 73.9 Wed 18:00 P2

**Adsorption of bifunctional methoxy butene on Si(001): the multiplicity of non-selective adsorption** — •Jannick Peters, Sophie Göbel, and Michael Dürr — Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany

Both, ether group and C=C double bond, adsorb on Si(001) via an intermediate state and with high reactivity. When combining these two functional groups in a bifunctional organic molecule, a variety of different adsorption configurations can be envisioned. However, selective adsorption via the ether group was found for allyl ethers on the Si(001) surface [1]. In the case of methoxy butene (MeBut), the functional groups are separated by an additional $CH_2$ group when compared to allyl ethers. Despite this seemingly small change in the molecules' structure, major differences in the reactivity on Si(001) were observed. At surface temperatures between 90 and 450 K, no selective reaction but a large variety of different adsorption configurations, which are bound either via ether cleavage, the C=C double bond, or both functional groups, was observed when studying intermediates and final products by means of XPS. Depending on the final configuration, the reactivity of the ether group was found to be either enhanced or reduced, which results in an increased temperature window for the reaction from intermediate to final state.

[1] T. Glaser, et al., J. Phys. Chem. Lett. 15, 7168 (2024).

O 73.10 Wed 18:00 P2

**Steel Mesh-Supported SNW-1/CsPbBr3 Nanocomposite: Photocatalyst for Sustainable Ammonia Production** — •Negin Khosroshahi and Vahid Safarifard — Iran University of Science and Technology, Tehran 16846-13114, Iran

The conversion of solar energy into chemical energy through photocatalysis is an important field of interest in green energy generation and environmental improvement. Nevertheless, its effectiveness currently falls short of expectations, primarily due to the issue of charge recombination. To address this challenge, the photocatalytic effect has become an optimistic approach for enhancing processes. In this research, we have developed a Steel Mesh-Supported SNW-1/CsPbBr3 nanocomposite by combining covalent-organic frameworks with metal halide perovskite. To gauge their effectiveness, the heterostructure was assessed by employing multiple characterization methods including XRD, IR, FESEM, DRS, EDX, VSM, PL, EIS, Zeta, and BET. After the composite's preparation and characterization, we examined its photocatalytic activity in nitrogen reduction. The SNW-1/MHP/Steel mesh nanocomposite exhibited exceptional performance in ammonia generation. These findings suggest that the SNW-1/MHP/Steel mesh nanocomposite holds promise as an environmentally friendly and cost-effective photocatalyst, capable of addressing the challenges of sustainable ammonia production. This study presents a promising method for identifying effective photocatalytic materials using mesh substrates to address environmental concerns.

# O 74: Poster Metal and Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Wednesday 18:00–20:00 Location: P2

O 74.1 Wed 18:00 P2

**Lithium adsorption on Cu(111) for anodeless lithium ion batteries** — •Darius Hübner — Universität Ulm, Institut für theoretische Chemie, Oberberghof 7, 89081 Ulm

Anodeless batteries in which the anode is created upon the first charging are of strong current interest as they avoid processing and cost concerns as well as lead to an increased safety. In order to contribute to the understanding of the the viability of copper charge collectors in anodeless Lithium ion batteries, we studied the deposition of lithium on a Cu(111) substrate using periodic density functional theory calculations.

We find that the lattice mismatch between lithium and copper leads to the formation of a fcc lithium structure with fewer atoms per layer than the copper substrate. Additionally, this lithium structure shows remarkably lower surface diffusion barriers compared to a standard bcc lithium surface. As an enhanced surface mobility is supposed to suppress dendrite growth, this suggests a reduced formation of dendrites in the initial steps of the anode formation.

O 74.2 Wed 18:00 P2

**Spin-State Switching of Indium-Pthalocyanine on Pb(100)** — Niklas Ide, Arnab Banerjee, •Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Kiel, Deutschland

Indium(III) phthalocyanine chloride, deposited on Pb(100), is investigated using a scanning tunnelling microscope at cryogenic temperatures. The chloride ions dissociate, leaving behind indium phthalocyanine (InPc), which is observed in two distinct configurations: the metal ion oriented either towards (↓) or away from (↑) the substrate. The study reveals isolated molecules and islands which exhibit a $\sqrt{65} \times \sqrt{65}, \mathrm{R} \pm 30^\circ$ superstructure, characterized by a unit cell containing four inequivalent molecules, one in the InPc↑ state and three in the InPc↓ state at different sites. Variations in the conductance spectra of the lowest unoccupied molecular orbital are observed, depending on the adsorption sites and azimuthal orientations of the complexes. Notably, only the InPc↑ molecules within the islands exhibit Shiba states, signifying the presence of a localized spin. Electron extraction allows for the conversion of both isolated complexes and molecules in islands from the InPc↑ to InPc↓ state. This transition is accompanied by a change in their spin state, as evidenced by the disappearance of the Shiba states.

O 74.3 Wed 18:00 P2

**On-surface fabrication of cesium tin halide nanostructures deviating from the perovskite $ABX_3$ structure** — Madad Abbasli, Dina Wilks, Carsten Busse, and •Robin Ohmann — University of Siegen, Siegen, Germany

We demonstrate that evaporation of the precursor molecules CsBr and $SnBr_2$ onto an atomically clean gold surface not only leads to the expected stoichiometric $CsSnBr_3$ structure, but also yields a range of other distinct structures. The experiments were conducted in ultra-high vacuum and investigated by scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). When deposited on Au(111), we observe a flower structure with hexagonal symmetry tentatively assigned to $Cs_2SnBr_6$, a ladder structure, a stripe pattern, a honeycomb structure, and a large square structure. The emergence of these structures depends on surface coverage - either submonolayer or multiple monolayers - and on the relative proportions of the two precursor molecules. In contrast, on Au(100) these structures are not observed, suggesting that the interface is playing a crucial role. The structures are compared with those formed by depositing either CsBr or $SnBr_2$ on Au(111). While a honeycomb structure can also be formed with $SnBr_2$ alone, the other structures bear no resemblence to either pure component. Thus, they are assigned to structures involving specific ratios of Cs, Sn and Br deviating from the standard $ABX_3$ structure. The structural variability underscores the importance of precise deposition conditions and interface selection in the fabrication of perovskite materials.

O 74.4 Wed 18:00 P2

**Band alignment at InP/$TiO_2$ interfaces from density-functional theory** — Isaac Azahel Ruiz Alvarado[1], Christian Dressler[2], and •Wolf Gero Schmidt[1] — [1]Universität Paderborn, Germany — [2]TU Ilmenau, Germany

The natural band alignments between indium phosphide and the titanium dioxide polymorphs rutile, anatase and brookite as well as amorphous titania are calculated from the branch point energies of the respective materials. Type-I alignment is predicted, irrespective of the type of titania interfacing with InP. The actual band offset may differ, however, from the natural band alignment depending on the microscopic structure of the interface. Supercell calculations are performed for the interface between P-rich InP(001) surface and amorphous titania thin films. The valence band offset increases substantially compared to the natural band alignment, while the conduction band offset is reduced, resulting in nearly aligned conduction bands. Depending on the interface properties, both type-I and type-II interfaces are observed in the simulations. The results show that with careful control of the microscopic interface structure and the atomic order of the titania film a very wide range of band alignments becomes accessible.

O 74.5 Wed 18:00 P2

**Structure of tellurium phases on Ni(111) and Ni(111)-(1 × 1)-2C (graphene)** — •Alexander Wegerich, Gwyn R. Thomas, Andreas Raabgrund, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Using quantitative LEED-IV analyses, STM and DFT, we examine Te on Ni(111) to understand the interactions and emerging structures. For $\Theta_{\mathrm{Te}} = 0.33\,\mathrm{ML}$ a $\left(3 \times \sqrt{3}\right)_{\mathrm{rect}}$-2Te superstructure is identified. For $\Theta_{\mathrm{Te}} = 0.40\,\mathrm{ML}$ this changes to a $\left(5 \times \sqrt{3}\right)_{\mathrm{rect}}$-4Te superstructure. As LEED-IV analyses reveal, these superstructures are identical to those that can be observed for the Te/Cu(111) system [1], albeit with different stacking and reduced Te-Metal bond length.

In addition, we also present our first results regarding Te on the well-known Ni(111)-(1 × 1)-2C (graphene) structure [2, 3]. The presence of Te reduces the thermal stability of the graphene on Ni(111). At annealing temperatures above 570 K the graphene begins to dissolve and structures for the Te/Ni(111) system emerge. In the course of our studies, we also determined the Ni(111)-(1 × 1)-2C (graphene) structure by LEED-IV analysis and obtained picometer accuracy by virtue of a low Pendry R-factor of R = 0.10.

[1] T. Kißlinger et al., Phys. Rev. B **104**, 155426 (2021)
[2] J. Lahiri et al., New J. Phys. **13**, 25001 (2011)
[3] Y. Gamo et al., Surface Science **374**, 61-64 (1997)

O 74.6 Wed 18:00 P2

**An atomistic analysis of the carpet growth of KCl across Ag(111) step edges** — •Anna Juliana Kny[1], Adam Sweetman[2], and Moritz Sokolowski[1] — [1]Clausius Institut für Physikalische und Theoretische Chemie, Universität Bonn, Germany — [2]School of Physics and Astronomy, University of Leeds, UK

Thin alkali halide (AH) films of 2-3 atomic layer thickness, grown on metal substrates, are widely used for studying decoupled molecules by scanning tunneling microscopy. For many combinations of AH and metal surface, a continuous growth of the AH layer across step edges of the substrate is observed, which is called carpet growth. Here, we report a first atomistic analysis of the layer distortions in the carpet growth region of KCl layers at Ag(111) step edges.[1] STM measurements were performed at room temperature and with Cl anions decorated W-tips which yield a high atomic resolution. We find that the AH layer distorts locally and in a non-uniform manner within a short lateral distance of four unit cells, when it grows across the Ag step. Furthermore, we find that the Ag(111) surface adapts to the AH layer, as the carpet growth is accompanied by a straightening of the Ag steps along the <110> direction and a splitting of higher Ag steps into multiple mono-atomic ones. These mono-atomic Ag steps allow for the carpet growth if the distance between them is larger than 13 Å, while a carpet growth across higher or closer Ag steps was not observed.[1]

Supported by the DFG through the research training group 2591, the Royal Society, and the ERC.

[1] A.J. Kny et al., J. Phys. Chem. Letters (2024), under revision.

O 74.7 Wed 18:00 P2

**Epitaxial growth of bismuthene-based transition metal compounds** — •Holger Diehm, Bing Liu, Simon Moser, Jörg Schäfer, and Ralph Claessen — Würzburg-Dresden Cluster of Excellence ct.qmat and Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany

This work explores the fabrication of alloy phases between bismuthene - a fully planar honeycomb structure of bismuth atoms on a silicon carbide (0001) substrate - and 3d transition metals (TMs).

Bismuthene is a promising candidate for quantum spin Hall (QSH) effect at room-temperature [1] that shows interacting 1D spin-polarized electrons in a metallic edge channel [2]. While topological protection of the edge channels can be lifted by edge coupling [3], interfacing it with ordered TM-rich phases could locally introduce magnetic moments. This provides a novel platform to explore the effects of broken time-reversal symmetry and its potential impact on the topological phase.

Our work focusses on epitaxially grown bismuthene, garnished with manganese, chromium or cobalt. While bismuthene on silicon carbide shows a rt(3) x rt(3) surface reconstruction in low energy electron diffraction (LEED), incorporation of transition metals causes an additional 3 x 3 phase. In addition, scanning tunneling microscopy (STM) is used to analyze the surface structure on an atomic level.

This study paves the way for both fundamental research and application-oriented development in spintronics.

[1] Science 357, 287 (2017); [2] Nat. Phys. 16, 47 (2020); [3] Nat. Commun. 13, 3480 (2022).

## O 75: Poster Focus Session Chemical Imaging for the Elucidation of Molecular Structure (joint session O/BP)

Time: Wednesday 18:00–20:00 Location: P2

O 75.1 Wed 18:00 P2

**Imaging of structure, conformation, and assembly of biological molecules by scanning probe microscopy (SPM)** — •Joshua Holloway, Márkó Grabarics, Banjamin Mallada, Alejandro Lynch Gonzalez, Lukas Eriksson, and Stephan Rauschenbach — University of Oxford, Oxford, UK

Direct imaging of (bio)molecules by scanning probe microscopy (SPM) is a powerful approach for molecular structure elucidation. Sample preparation presents a challenge: an analyte must be taken into the gas phase, and intactly deposited on the sample surface. Because many biological molecules we wish to study are incompatible with sublimation, we employ electrospray ion beam deposition (ES-IBD). A novel, custom-built deposition stage extending a commercial mass spectrometer (Thermo Fisher Q Exactive UHMR) allows for mass-filtered, soft-landed deposition onto atomically flat metal crystals for high-performance SPM imaging.

Here we present the workflow of mass spectrometry, selection, deposition, and imaging for several examples of biological molecules. In particular we explore the imaging of molecular assemblies of biomolecules with large and small ligands, formed in the gas-phase and/or on the surface.

## O 76: Poster Focus Session Atomic Scale Investigation of Magnetic 2D Materials

Time: Wednesday 18:00–20:00 Location: P2

O 76.1 Wed 18:00 P2

**Unconventional magnetic response in epitaxial-grown single-layer $Cr_2S_3$-2D** — •Affan Safeer[1], Calisa Carolina Oliveira[2], Mahdi Ghorbani-Asl[3], Jörg Schöpf[1], Wouter Jolie[1], Amilcar Bedoya-Pinto[2], Arkady V. Krasheninnikov[3], Thomas Michely[1], and Jeison Fischer[1] — [1]Universität zu Köln, Köln, Germany — [2]University of Valencia, Paterna, Spain — [3]Institute of Ion Beam Physics and Materials Research, Dresden, Germany

We studied the magnetic ordering in epitaxially-grown single-layer $Cr_2S_3$-2D on Gr/Ir(110) using X-ray magnetic circular dichroism (XMCD), scanning tunneling microscopy (STM) and spectroscopy (STS). Prior characterization of the 2D material structure via low-energy electron diffraction (LEED), STM, and density functional theory (DFT) calculations confirmed that single-layer $Cr_2S_3$-2D has a NiAs-type structure. DFT calculations further predicted that the ground state could be either A-type antiferromagnetic or ferromagnetic, depending on the Hubbard parameter. Differential conductance STS measurements as a function of the out-of-plane magnetic field at 1.7 K show a hysteresis behavior with a switching field of about 4T, indicating a ferromagnetic ordering. In contrast, XMCD measurements on the same sample revealed no signal, indicating zero net magnetic moment, suggesting antiferromagnetic behavior.

O 76.2 Wed 18:00 P2

**Atomically thin $MnBr_2$ grown by molecular-beam epitaxy on graphene/Ir** — Oktay Güleryüz, Affan Safeer, Nicolas Georgopoulos, Thomas Michely, and •Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

We report on the growth of potentially magnetic manganese dibromide ($MnBr_2$) films on graphene/Ir substrates using molecular-beam epitaxy. $MnBr_2$ is evaporated as a single compound from an effusion cell onto the graphene/Ir. Low-electron energy diffraction analysis reveals that the hexagonal lattice constant of $MnBr_2$ amounts to $0.390 \pm 0.005$ nm, consistent with calculated 0.3885 nm and bulk 0.3873 nm values.

Our scanning tunneling microscopy study reveals that the best growth conditions to form large, compact monolayers involve deposition at elevated temperatures (400 K). Growth at low temperature on graphene/Ir(110) leads to the formation of small islands with a distribution of orientations. A new moiré superstructure is formed, which reflects the interaction of the $MnBr_2$ lattice with the corrugated graphene/Ir(110) moiré.

Low-temperature scanning tunneling spectroscopy at 1.7 K of monolayer $MnBr_2$ further reveals a significant band gap of approximately 5 eV. Additionally, isolated polarons are observed, which can be manipulated, created, and destroyed by the STM tip.

O 76.3 Wed 18:00 P2

**The Nickelocene as an STM Atomic-Spin Sensor via cotunnelling theory** — •Andres Pinar Sole[1,2], Manish Kumar[1], Diego Soler-Polo[1], Oleksandr Stetsovych[1], and Pavel Jelinek[1] — [1]Czech Institute of Physics, Cukrovarnicka 10, Prague 6, 16200 (Czech Republic) — [2]Center for Quantum Nanoscience (QNS) Research Cooperation Building Ewha Womans University, 03760 Seoul, (Republic of Korea)

Functionalization of a scanning microscopy probe with a single nickelocene attached to the tip allows reproducible spin-sensitive measurements of magnetic systems on surfaces. As a S=1 molecule, the triplet ground state of the nickelocene tip gives rise to a inelastic electron spin-flip excitation which changes upon interactions with spin systems on the surface. Some advantages of nickelocene functionalization compared to spin-polarized tips include tip passivation, enabling data acquisition at close tip-sample distances and well defined spin and tip apex. These features enable us to determine the local spin moment on the surface with atomic-scale precision.

While the interactions between the nickelocene spin and the magnetic centers has been modelled using a two-site Heisenberg Hamiltonian, we complement it to include the tunnelling current as an electronic transport phenomenon via cotunneling theory. It allows understanding the absence of transitions that are not allowed according to the selection rules or have relatively weaker intensity. We cover S = 1/2, 1, and 3/2 systems, as well as 2D magnetic materials and compare the simulations with experimental results.

# O 77: Poster Vacuum Science Technology: Theory and Applications

Time: Wednesday 18:00–20:00 Location: P2

O 77.1 Wed 18:00 P2

**An apparatus of preparing frozen solution samples for ultra-high vacuum experiments** — •Jiadong Guo, Xinmeng Liu, and Ying Jiang — International Center for Quantum Materials, School of Physics, Peking University, Beijing, China

Here we develop an apparatus for preparing frozen solution samples, which can be characterized by surface science techniques under ultra-high vacuum (UHV) condition. When a temperature-variable substrate is approached to contact the frozen solution at 77 K, the surface of the frozen solution is locally melted and then refreeze with the substrate. By detaching the substrate from the frozen solution in high vacuum, the frozen solution is cleaved and transferred onto the substrate. Applying this method, we demonstrate transferring NaCl and $LiNO_3$ frozen solutions onto the Au substrate, and directly image the crystallization of NaCl and $LiNO_3$ using atomically resolved atomic force microscopy (AFM) in UHV at 5 K.

This apparatus provides a new approach to transfer solution samples in their glassy states into the UHV environment while maintaining the cleanliness of the samples, laying the foundation for further research related to solution environment, such as crystallization, hydration, chemical reaction, materials synthesis and bioimaging.

O 77.2 Wed 18:00 P2

**Investigating Nanoscale Hydrophobic Polymer Coatings for the use in the Einstein Telescope** — •Maike Kühler, Achim Stahl, Charlotte Benning, and Oliver Pooth — III. Physikalisches Institut B, RWTH Aachen

With 120 km pipes of 1m diameter, the ultra-high vacuum (UHV) system of the Einstein Telescope is going to be one of the largest vacuum systems in existence. It will need an enormous input of innovation and optimization. This work explores superhydrophobic coatings for the vacuum chambers of the Einstein Telescope. Hoping to achieve faster pumpdown times and eventually lower bake out temperatures to reach sufficient pressure regimes. This poster presents a coating based on reactive silyl anchor units and functionalised with a long perfluoropolyether/organofluorine chain. The coating has been investigated for its performance and compatibility with UHV conditions. Its compatibility with the vacuum system of the Einstein Telescope was evaluated through molecular flow simulations.

O 77.3 Wed 18:00 P2

**Tritium Induced Exchange Reaction of Hydrogen Isotopes** — •James O'Callaghan, Robin Grössle, Simon Niemes, and Robin Holzwarth — Tritium Laboratory Karlsruhe (TLK), Institute of Astroparticle Physics (IAP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Tritium (T), the heaviest isotope of hydrogen, is used for experiments in astro-particle physics and is essential as fuel for fusion reactors. It comes with many challenges due to its radioactivity. Isotopic exchange is one such challenge, Hydrogen-1 (H) and Deuterium (D) can be left in an idealised vessel and will practically not react with each other; the concentrations of H2, D2 and HD will remain unchanged and will not reach the thermal equilibrium in practical time scales. This is not the case with tritium. In the presence of tritium, the radioactive decay induces chemical reactions and therefore the concentrations will shift towards the chemical equilibrium. Most prominently in a fusion reactor context, starting with mixtures of homonuclear molecules (H2, D2, T2), the production of potentially undesirable heteronuclear molecules (HD, HT and DT) up to the chemical equilibrium is facilitated by the decay of tritium. This needs to be understood for designing fuel cycle components for a fusion reactor. In this contribution first efforts for a data driven development of an empirical model to describe the reactions rates in tritiated mixtures is given.

# O 78: Overview Talk Manish Garg

Time: Thursday 9:30–10:15 Location: H24

**Topical Talk** O 78.1 Thu 9:30 H24

**Imaging Electronic and Atomic Motion in Molecules** — •Manish Garg — Max Planck Institute for Solid State Research, Heisenbergstrasse 1, Stuttgart 70569

The capability to capture electronic and atomic motions at their natural length (Ångstrom-scale) and time-scales (attoseconds to femtoseconds) is a long-standing goal in modern science. In my talk, I will show you how electron dynamics in molecules can be locally probed with angstrom-scale spatial resolution and sub-femtosecond temporal resolution simultaneously, at the single orbital-level with the help of a scanning tunnelling microscope (STM), defying the previously established fundamental space-time limits [1-3].

Quantum decoherence of the excited electronic states and dipole-dipole interactions between molecules can now be imaged in real-space and real-time. We have recently imaged electronic excitation transfer dynamics between donor and acceptor kind of molecules. Excitons locally excited in a donor molecule exchanges energy by coherent dipole-dipole interaction with a neighboring acceptor molecule [4].

Atomic motions in a single molecule can be directly imaged by realizing coherent anti-Stokes Raman spectroscopy in an STM [5-8]. These recent developments pave the way towards direct real space-time imaging of chemical reactions and phase transformations in two-dimensional materials.

# O 79: Ultrafast Electron Dynamics III

Time: Thursday 10:30–12:30 Location: H2

O 79.1 Thu 10:30 H2

**Hybrid Exciton Orbital Tomography in 2D-organic interfaces** — •Christian Simon Kern[1], Michele Capra[2], Marco Gruenewald[3], Torsten Fritz[3], Mirko Cinchetti[2], Peter Puschnig[1], and Giovanni Zamborlini[1] — [1]Institute of Physics, University of Graz, Austria — [2]Department of Physics, TU Dortmund University, Germany — [3]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Organic molecules adsorbed on semiconducting 2D substrates pose an interesting class of interfaces for optoelectronic applications. Here we investigate the interface of pentacene and a transition metal dichalcogenide layer with many-body perturbation theory. In particular, we compare those results to optical spectroscopy and demonstrate the connection of excitons to their experimentally observable photoemission signatures in pump-probe spectroscopy. The latter approach— exciton photoemission orbital tomography [1]—especially allows for the unambiguous characterization of the excitons' hole and electron configuration, and is extended to the case of hybrid interlayer excitons.

[1] C. S. Kern, A. Windischbacher, and P. Puschnig, Photoemission orbital tomography for excitons in organic molecules, PRB 108, 085132 (2023)

O 79.2 Thu 10:45 H2

**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 79.3 Thu 11:00 H2

**Exciton wave function signatures from time-resolved photoemission tomography of an organic molecular layer** — •Siegfried Kaidisch[1], Marcel Theilen[2], Monja Stettner[3], Eric Fackelman[3], Galit Cohen[4], Amir Kleiner[4], Christian Simon Kern[1], Andreas Windischbacher[1], Sivan Refaely-Abramson[4], Frank Stefan Tautz[3], Ulrich Höfer[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]Fachbereich Physik, Philipps-Universität Marburg — [3]PGI-3, FZ Jülich & RWTH Aachen University — [4]Weizmann Institute of Science, Israel

Oriented layers of organic molecules adsorbed on passivated metal surfaces are a promising class of interfaces for studying electron dynamics at femtosecond timescales. In particular, time-resolved photoemission tomography promises to reveal information about the electron distribution in optically excited states. Using the example of sexithiophene (6T) multilayers adsorbed on Cu(110)-p(2x1)O, we observe photoemission patterns for the low-energy excited states. These measured momentum maps exhibit signatures that cannot be explained by a mere population of the lowest unoccupied molecular orbital of 6T. To analyze the source of these features, we perform GW/BSE (Bethe-Salpeter equation) calculations on multiple levels of theory (gas-phase, cluster, embedded and periodic calculations). Using the framework of photoemission orbital tomography for excited states, we also simulate the photoemission patterns and thereby shed light on the nature of the exciton wave function of the lowest optically allowed state.

O 79.4 Thu 11:15 H2

**Quenching Strong-Field Recollisions at Nanotapers with Strong Bias Fields** — •Rasmus Lampe, Germann Hergert, and Christoph Lienau — Institut für Physik, Carl-von-Ossietzky Universität, 26129 Oldenburg, Germany

Recollisions of intensively accelerated electrons with the parent are a well-known effect in strong-field photoemission of electrons, leading to photoemission spectra showing a recollision plateau with a cut-off energy of ten times the ponderomotive energy. It has recently been demonstrated that such a recollision plateau also arises in multiphoton photoemission from metallic nanostructures, showing that recollisions are much more fundamental to photoemission than anticipated [1].

We analyze electron recollisions from strongly biased tungsten nanotapers illuminated by few-cycle near-infrared laser pulses. We demonstrate significant changes in the photoelectron spectra in the strong-field regime by applying static electric fields on the order of the optical near-field driving the photoemission. A continuous transition of a horizontal recollision plateau into triangularly shaped spectra is observed.

Stronger static fields increase the acceleration of the electrons away from the apex, such that the ponderomotive acceleration by the near-field is not sufficient to drive the electrons back to the surface, ultimately suppressing recollisions. This enables the control of the electron motion with bias fields, which has an immediate importance for ultrafast low-energy electron microscopy allowing to maintain few fs time resolution of the electron beam over mesoscopic distances.

[1] B. Bánhegyi et al., Phys. Rev. Lett. 133, 033801 (2024)

O 79.5 Thu 11:30 H2

**Time-resolved photoemission orbital tomography of 6T on Cu(110)-(2×1)O** — •Marcel Theilen[1], Monja Stettner[2], Eric Fackelman[2], Francois C. Bocquet[2], Alexa Adamkiewicz[1], Sarah Zajusch[1], Siegfried Kaidisch[3], Christian Kern[3], Robert Wallauer[1], Peter Puschnig[3], F. Stefan Tautz[2], and Ulrich Höfer[1,4] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [3]Institut für Physik, Universität Graz — [4]Fachbereich Physik, Universität Regensburg

For ordered molecular layers, photoemission orbital tomography (POT) is a powerful technique for imaging the electron distribution of molecular orbitals in momentum space. When combined with laser pump-probe techniques, time-resolved photoemission orbital tomography (tr-POT) offers the ability to track the population dynamics of the excited molecular states on a femtosecond time scale[1].

In this talk, I will discuss our recent results obtained through tr-POT for three distinct, well-ordered layers of sexithiophene (6T) on a Cu(110)-(2×1)O surface: a monolayer, a bilayer and a multilayer. The focus will primarily be on the dynamics of the populated 6T LUMO via an optically HOMO-LUMO transition. For instance, a comparison between the individual layers reveals a significant extension of the LUMO lifetime with increasing layer thickness. Specifically, we find that the lifetime for the monolayer is less than 50 fs, while it increases to more than 600 fs for the multilayer.

[1] R. Wallauer *et al.*, Science **371**, 1056 (2021).

O 79.6 Thu 11:45 H2

**Understanding the ultrafast electron dynamics and CDW transition in LaTe$_3$ using machine learning** — •Gesa Siemann[1], Davide Curcio[1], Paulina Majchrzak[1], Charlotte Sanders[2], Jenny Rigden[2], Yu Zhang[2], Deepnarayan Biswas[3], Leslie Schoop[4], Emma Springate[2], 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]Department of Chemistry, Princeton University, USA

The rare-earth tritelluride LaTe$_3$ hosts a unidirectional charge density wave (CDW) with a high transition temperature of 670 K. Recently, it has been suggested that exposing the system to a short light pulse not only suppresses this primary CDW but also induces a second CDW in the perpendicular direction[1]. An open question is, how these structural dynamics affect the electronic structure, and if fingerprints of the second CDW can be found in corresponding data obtained by time- and angle-resolved photoemission spectroscopy. Here, we explore this question, studying the frequency-dependent coherent response of the system, and the time-dependent evolution of the Fermi surface topology, which we compare to predictions by a simple tight-binding model. We support our analysis using $k$-means clustering, a machine learning technique, in order to identify different dynamics throughout the Brillouin zone. This reveals varying relaxation times across the Fermi surface, as well as multiple frequencies that can be ascribed to coherent excitations. [1]A. Kogar *et al.*, *Nat. Phys.* 16, 159*163 (2020).

O 79.7 Thu 12:00 H2

**Following charge-transfer between plasmonic NPs and adsorbed molecules by time-resolved IR spectroscopy** — •Daniel Sandner[1], Katrin Schulz[1], Andrei Stefancu[2], Reinhard Kienberger[1], Emiliano Cortes[2], and Hristo Iglev[1] — [1]Lehrstuhl für Laser- und Röntgenphysik E11, TUM, James-Franck Str 1, 85748 Garching — [2]Fakultät für Physik, LMU München

Plasmonic Nanoparticles can efficiently convert light in a broad range into hot charge carriers, which can be subsequently transferred to molecules or semiconductors for photocatalytic processes. The role of charge-carrier-mediated or thermal reaction pathways is still under debate. Here, we use time-resolved IR spectroscopy between 1200-3000 cm-1 as a sensitive probe for free charges and study the dynamics of different molecules attached to silver NPs. Charge transfer is only observed for resonant excitation of the plasmon resonance and in the presence of attached molecules. Furthermore, we find a correlation between the lifetime of transferred charges and the chemical reactivity.

O 79.8 Thu 12:15 H2

**Ultrafast Photoexcitation of Semiconducting Photocathode Materials: An Ab Initio Study** — •Hilde Bellersen, Michele Guerrini, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg, Germany

Cs-based semiconductors like Cs$_3$Sb and Cs$_2$Te are currently used as photocathode materials in particle accelerators. Their performance as electron sources critically depends on their response to the intense laser radiation impinging them. In this work, we investigate from first principles the time-dependent response of Cs$_3$Sb and Cs$_2$Te to ultrafast laser pulses of varying intensities, ranging from 1 GW/cm$^2$ to 100 TW/cm$^2$. Nonlinear effects, including high harmonic generation and multiphoton absorption, emerge at thresholds of 400 GW/cm$^2$ for Cs$_3$Sb and 500 GW/cm$^2$ for Cs$_2$Te. Beyond these intensities, the energy uptake and number of excited electrons saturate, with renewed increases observed beyond 10 TW/cm$^2$. These findings provide new insights into the nonlinear optical properties of Cs$_3$Sb and Cs$_2$Te, contributing to the optimization of these materials for the development of next-generation photoinjectors.

## O 80: Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties I

Time: Thursday 10:30–12:30 Location: H4

O 80.1 Thu 10:30 H4

**CISS in single heptahelicene molecules on Fe bilayers on W(110)** — •Daniel E. Bürgler[1], Mohammad Reza Safari[1], Frank Matthes[1], Karl-Heinz Ernst[2], and Claus M. Schneider[1] — [1]Peter Grünberg Institut, Forschunszentrum Jülich, Germany — [2]Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600, Dübendorf, Switzerland

We reproduce and extend our single-molecule studies of CISS [1,2] to an alternative substrate system. Heptahelicene molecules are sublimed onto a multi-domain Fe bilayer film on W(110) instead of single-domain Co bilayer nanoislands on Cu(111). Using spin-polarized low-temperature scanning tunneling microscopy, the current flow through single *(M)*-enantiomers chemisorbed on neighboring and oppositely magnetized domains of the Fe bilayer film is mapped in the constant-height mode, where the tip is scanned at constant height above the Fe surface. The CISS magnetoresistance reaches up to 18% at 5 K and shows a strong dependence on the bias voltage. A comparison is drawn with the data obtained on Co nanoislands.

[1] M.R. Safari, F. Matthes, V. Caciuc, N. Atodiresei, C.M. Schneider, K.-H. Ernst, D.E. Bürgler. Adv. Mater. **36**, 2308666 (2024)
[2] M.R. Safari, F. Matthes, C.M. Schneider, K.-H. Ernst, D.E. Bürgler, Small **20**, 2308233 (2024)

O 80.2 Thu 10:45 H4

**STM topography and photoluminescence of three different Eu complexes** — •Adrian Ebert[1], Lukas Gerhard[1], Julia Feye[2], Senthil Kumar Kuppusamy[3], Mario Ruben[3], Peter Roesky[2], and Wulf Wulfhekel[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute for Organic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

We explore the self-assembly and luminescence properties of three distinct Europium (Eu) complexes *Eu(tta)$_3$(H$_2$O)$_2$ , Eu(btfa)$_3$(bpy) , and Eu(tta)$_3$(bpy) * on a Au(111) surface. Utilizing Scanning Tunneling Microscopy (STM), we explore the molecular topography and the ordered structures formed by these complexes, providing insight into their surface interactions. The Europium Eu$^{3+}$ ion, a member of the lanthanide series, is renowned for its unique photophysical properties, particularly its sharp emission lines and long-lived luminescence, which make it a valuable component in light-emitting devices, bio-imaging, and sensing applications.

O 80.3 Thu 11:00 H4

**First-Principles Modeling of Mixed-Dimensional Heterostructures: A Path Forward** — •Jannis Krumland and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg

Inorganic/organic interfaces between transition-metal dichalcogenides and organic adsorbates are promising candidates for future optoelectronic applications, leveraging and combining the unique strengths of the two different types of materials. The first-principles description of such interfaces, however, remains challenging because methods based on density-functional theory are unreliable for their simulation [1]. This is a result of the mixed dimensionality of the interface, with molecules being zero-dimensional while surfaces are two-dimensional. The mixed dimensionality moreover poses challenges in the analysis of the results, as molecules are usually described in terms of energy levels, whereas surfaces are characterized by band structures. Here, we present a methodological study establishing pragmatic yet accurate simulation approaches for the calculation of energy-level alignments [2]. In addition, we highlight unfolding techniques as a key tool for gaining a deeper understanding of the interactions and hybrid-state formation occurring at such interfaces [3].

[1] J. Krumland and C. Cocchi, Phys. Stat. Sol. A 221, 2300089 (2024)
[2] J. Krumland and C. Cocchi, J. Phys. Chem. Lett. 15, 5350-5358 (2024)
[3] J. Krumland and C. Cocchi, Electron. Struct. 3, 044003 (2021)

O 80.4 Thu 11:15 H4

**Photo-induced force microscopy of organic molecules on thin van der Waals substrates** — •Markus Kratzer[1], Mohamad Khan[1], Simon Leitner[1], Aleksandar Matkovic[1], Olivier Siri[2], Conrad Becker[2], and Christian Teichert[1] — [1]Chair of Physics, Montanuniversität Leoben, Franz-Josef Straße 18, 8700 Leoben, AUT — [2]Aix Marseille Univ., CNRS, Cinam, 13288 Marseille, FGrance

Photo-induced force microscopy (PiFM) is an atomic force microscopy based technique for obtainiung infrared spectroscopic data with a spatial resolution down to a few 10 nm. Here, we utilized PiFM to investigate nano and microstructures comprising small organic molecules like para-hexaphenyl or dihydro-tetraaza-acene (DHTA7) on exfoliated thin layers of van der Waals materials as hexagonal boron nitride (hBN). It is notices that the PiFM spectra systematically vary with van der Waals substrate thickness. Further PiFM spectra of upright standing molecular structures and flat lying structures are copared. PiFM turned out to be sensitive even for single molecular layers, which are only about 2 nm thick. Similarities and differences between thin film and bulk infrared data are discussed.

O 80.5 Thu 11:30 H4

**Engineering Optical Properties through Polymorphism** — •Nina Kainbacher[1,2], Peter Puschnig[1], and Oliver T. Hofmann[2] — [1]Institute of Physics, University of Graz, Austria — [2]Institute of Solid State Physics, Graz University of Technology, Austria

Molecular monolayers on a supporting substrate can order in different configurations, i.e. polymorphs. Owing to variations of the intermolecular coupling between the transition dipole moments, we expect that different polymorphs exhibit also distinctly different optical properties due to changes in transition energies and oscillator strengths. In this study, we computationally study the impact of polymorphism of organic molecular monolayers on optical absorption spectra. Specifically, we investigate influencing factors, such as geometric distortions upon adsorption, interactions between transition dipole moments, changing selection rules due to the symmetry of different polymorphs, and particularly, effects arising from the potential delocalization of the wave functions. As an example, we predict the polymorphism of the dipolar organic molecule nitro-pyrene-amine on NaCl(100) using machine learning-based structure search and calculate its optical properties based on density functional theory and the RPA approximation. Specifically, we find two distinctly different polymorphs, where the excitation energies differ by approximately 0.2 eV which we attribute to a combination of the above-mentioned effects.

O 80.6 Thu 11:45 H4

**Imaging the occupied states of multilayers of $\alpha$-sexitiophene (6T) on Cu(110)-p(2x1)O using orbital tomography** — •Monja Stettner[1,2], Andrey Matetskiy[1], Eric Fackelman[1,2], Siegfried Kaidisch[3], Serguei Soubatch[1], François C. Bocquet[1], Peter Puschnig[3], Christian Kumpf[1,2], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), FZ Jülich, Germany — [2]RWTH Aachen University, Germany — [3]Institute of Physics, University of Graz, Austria

Deposition of $\alpha$-sexithiophene (6T) on an oxygen-reconstructed Cu(110)- p(2x1)O surface results in a well ordered, close-packed monolayer structure, and at higher coverages in layer-by-layer growth. Note that even beyond a monolayer, 6T retains its orientation along the [001] direction of Cu. We investigated samples with coverages of up to eight layers using ARPES and - in particular - orbital tomography. For the latter, experimental momentum maps are compared to simulated maps which are calculated for a single free molecule and for extended layers of 6T. We found a good resemblance for several occupied molecular states, e.g., the HOMO. However, in the binding energy range of several deeper orbitals, the momentum maps clearly show signatures of a sizable intermolecular dispersion that cannot be explained by a superposition of the single gas phase maps. The orbitals rather form dispersing bands, which indicates a significant intermolecular hybridization.

O 80.7 Thu 12:00 H4

**Electronic structure of molecular and crystalline benzene on an $MoS_2$ monolayer** — •Jan-Philipp 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 molecular benzene and its bulk crystal as prototypical systems.

We use DFT (GGA) and DFT-D3 to determine the most stable adsorption position of both the molecule and the bulk crystal on $MoS_2$. Subsequently, we use many body perturbation theory to calculate the electronic spectrum of the adsorbate system and its individual components ($MoS_2$ and the benzene molecule/crystal) in order to investigate the effect of the molecule on the $MoS_2$ electronic and optical spectrum.

O 80.8 Thu 12:15 H4

**Contact-dependent electronic properties of anthracene-$MoS_2$ heterostructures** — •Hsin-Mei Ho and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Flexible nanodevices composed of atomically thin layers have revolutionized fundamental and applied sciences. Based on density functional theory (DFT), we consider the organic-inorganic heterostructures: anthracene molecules adsorbed on monolayer $MoS_2$. Our investigations of the adsorption geometries and the energy band dispersions demonstrate that the contact between the organic and inorganic layers greatly affects the electronic properties. Anthracene thin films give rise to different shifts of the frontier energy levels, and consequently, variations in the band alignments when the molecules are in the perpendicular and parallel orientations on $MoS_2$. As anthracene is known for ordered structures when grown on substrates, we find in the present study that the bandgap of an anthracene film reduces when the interactions between molecules increase. This suggests that how the molecules are packed also plays a critical role. Our study provides detailed insights regarding the advances of oligoacene-TMDs layers for both theoretical and experimental sides.

## O 81: Heterogeneous Catalysis III

Time: Thursday 10:30–12:30 Location: H6

O 81.1 Thu 10:30 H6

**Cu Oxide Nanoparticles for Virus Inactivation** — •Daniel Silvan Dolling[1,2], Miguel Blanco Garcia[1,2], Mona Kohantorabi[1], Mohammad Ebrahim Haji Naghi Tehrani[1,2], Jan-Christian Schober[1,2], Ming-Chao Kao[1,2], Jagrati Dwivedi[1], Arno Jeromin[1], Thomas F. Keller[1], Olof Gutowski[3], Dimitry V. Novikov[3], Andreas Stierle[1,2], and Heshmat Noei[1] — [1]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, Jungiusstraße 11, 20355 Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

$TiO_2$ is known to inactivate SARS-CoV-2 photocatalytically under UV light. Recently, it has been shown that Cu oxide on Titania shifts the photoactivty into the visible light region. The specific oxidation state of Cu is paramount for the photocatalyst efficiency. Here, we use single crystalline $TiO_2$ to investigate the effects of growth conditions of Cu nanoparticles (NPs). To this cause, we employ X-ray diffraction (XRD) and scanning electron microscopy (SEM), revealing a temperature-dependent morphology. Subsequently, we analyze the short- and long-term oxidation behavior with X-ray photoelectron spectroscopy (XPS) and scanning Auger microscopy (SAM). Finally, we investigate the interaction of the NPs with asparagine amino acid using reflection-absorption infrared spectroscopy (IRRAS) and grazing-incidence small-angle scattering (GISAXS).

O 81.2 Thu 10:45 H6

**Charting Catalysis: Unveiling Regime Boundaries in Kinetic Phase Spaces Through Concentration Profiles** — •Maryke Kouyate, Gianmarco Ducci, Frederic Felsen, Christian Kunkel, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

In an industrial context, optimizing process variables is a critical step in ensuring optimal performance of catalytic reactors. Selecting the relevant process variables not only aids in meeting precise requirements but also in streamlining reactions and thus saving time and costs. Robust kinetic rate laws capable of accurately describing experimental data allow for predictive modelling in reactor design, optimization, and control. Specialized profile reactors efficiently yield the required data to derive kinetic models by providing access to spatio-temporally resolved chemical information along the reactor axis. Depending on the range of experimental conditions and the catalytic reaction, the kinetic phase space can exhibit sub-regions of smooth kinetic behavior, separated by transitional regions characterized by sudden qualitative changes of the kinetic behavior. These kinetic phase transitions carry important information about the catalytic reaction network. To pinpoint distinct sub-regions and corresponding models within a kinetic phase diagram, we propose an automated system capable of systematically exploring the design space. This algorithm manages the experimental reactor and iteratively suggests new experiments through model-based design of experiments.

O 81.3 Thu 11:00 H6

**Mechanistic Probes for Photocatalysis: Gas Phase Reactions of Tertiary Alcohols on Titania in a Micro-Photoreactor** — •Martin Tschurl[1], Clara Aletsee[1], Paula Neumann[1], Ib Chorkendorff[2], 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

The lack in mechanistic understanding still hinders the rational design of efficient photocatalyst for various applications. To gain more comprehensive insights into the fundamental effects in photocatalysis, we analyze the gas phase photoreactions of tertiary alcohols on titania powder in a micro-photoreactor in a well-defined environment under the exclusion of oxygen. The parallels of the observed reaction properties to studies performed on a rutile single crystal in vacuum suggest similar mechanistics, which is in contrast to the generally assumed reaction model under such conditions. Furthermore, the time resolution of the micro-reactor setup allows the determination of the alcohol surface coverage, which excludes the existence of liquid films and evidences a gas phase reaction. In addition to the scientific insights on photocatalysis on titania, these results demonstrate the use of tertiary alcohols as suitable probe reactants for mechanistic studies.

O 81.4 Thu 11:15 H6

**Selectivity trends in CO hydrogenation over transition metal surfaces** — •David Degerman[1,2], Patrick Lömker[1], Markus Soldemo[1], Fernando Garcia-Martìnez[3], Robin Yoël Engel[1,2], Martin Beye[1,2,3], and Anders Nilsson[1,2] — [1]Department of Physics, Stockholm University, 114, 21, Stockholm, Sweden — [2]WISE - Wallenberg Initiative Materials Science for Sustainability, Department of Physics, Stockholm University, 114, 21, Stockholm, Sweden — [3]Deutsches Elektronen Synchrotron, DESY, Photon Science, Notkestraße, 22607, Hamburg, Germany

Understanding the selectivity of heterogeneously catalyzed CO hydrogenation is increasingly important for the transition towards a sustainable chemical industry. While theoretical studies yielded a model based on the competition of various elementary surface reactions, we need experimental observation of the surface's chemical state to verify the mechanistic origin of the selectivity. Here, we compare in-situ x-ray photoelectron spectra over operating single crystal catalysts (200 to 325 °C, 150 mbar) of Fe, Rh, Ni, Co and Cu and infer from the observed trends which mechanistic steps decides the product distribution for each material. In particular, we find that the chemisorption energies of C and O (commonly used descriptors for activity and selectivity) qualitatively predicts the rate-limiting step of catalysts, but fails when the reaction mechanism of Ni and Fe is fundamentally altered due to reaction-induced carburization. This work emphasizes that the complete chemical overview provided by photoemission spectroscopy is required to understand the selectivity of CO hydrogenation.

O 81.5 Thu 11:30 H6

**Exploration of Explicit Solvation Effects in Heterogeneous Catalysis Using Machine Learning Interatomic Potentials** — •Maciej Baradyn and Johannes T. Margraf — University of Bayreuth

The presence of solvent affects many aspects of modeling elementary reactions involved in heterogeneous catalysis, such as stabilization of adsorbed species, the nature of interaction with the surface, as well as energetics and reaction rates, to name just a few. Unfortunately, treating solvent effects in atomistic simulations is a great challenge, since the solvent adds many additional degrees of freedom to the calculation. In first-principles calculations, implicit solvation models are often used to approximately include these effects with moderate computational effort. However, they do not take into account the explicit solvent-surface and solute-solvent interactions, and are therefore known to fail, e.g. when hydrogen bonding is important. More importantly, the solvent molecules can sometimes play a decisive role in the reaction's mechanism (e.g. as proton shuttles), which cannot be captured by implicit models, where solvent is treated as a continuous medium. In this contribution, we explore the efficiency of machine learning potentials based on the MACE-MP-0 foundation model for describing explicit solvation at catalytic interfaces. These potentials are used to capture the kinetic and thermodynamic parameters of small organic molecules interacting with metallic surface in an explicit water bath. Implications for our understanding of the underlying catalytic reaction network and improved design of catalysts will be discussed.

O 81.6 Thu 11:45 H6

**Reducibility of Sm-doped ceria islands on Ru(0001)** — •Raquel Sanchez-Barquilla, Rudi Tschammer, Lars Buss, Carlos Morales, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Germany

The interaction between metal and oxide is critical when considering the hydrogenation of $CO_2$ to hydrocarbons. In this context, the inverse oxide/metal catalysis architecture allows for achieving better catalytic performance due to strong oxide-metal interactions. In particular, in cerium-based inverse catalyst systems, the $Ce^{3+}$ cations have been demonstrated to play an active role in methanol synthesis, suggesting that the activity can be enhanced by promoting those through alloying with trivalent, catalytically active rare-earth metals, such as Sm. Here, we present a low-energy and X-ray photoemission electron microscopy (LEEM/XPEEM) investigation that shows how the reducibility of $CeO_2(111)$ islands on Ru(0001) is highly enhanced when doped with Sm. After post-annealing with Sm, intensity-voltage (I-V) LEEM curves show an immediate reduction of the islands at the surface. Exposure to low $H_2$ pressures efficiently reduces the islands to a (3×3) superstructure formed by ordered oxygen vacancies, as evidenced by characteristic IV-LEEM spectra and low-energy electron diffraction patterns. Furthermore, annealing at high temperatures shows the further reduction of the Sm-ceria islands, with features characteristic of the hexagonal $Ce_2O_3(0001)$ phase. While this reduction takes about one hour for pure ceria, this transition is virtually immediate for the Sm-doped ceria islands at comparable conditions.

O 81.7 Thu 12:00 H6

**Interaction of single cobalt co-catalyst atoms with the $SrTiO_3(001)$ surface** — •Aji Alexander[1], Pankaj Kumar Samal[1], Llorenç Albons[1], Jan Škvára[1], Dominik Wrana[2], Viktor Johánek[1], Josef Myslivecek[1], and Martin Setvin[1] — [1]Department of Surface and Plasma Science, Charles University, Prague, Czech Republic — [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland

Perovskite surfaces attract attention in the catalysis community due to their promising chemical properties, ability to separate electron-hole pairs for light harvesting, and ferroelectricity in various phases. Understanding metal clusters, specifically their electronic structure and atomic utilization efficiency, is crucial for developing more efficient and sensitive catalysts.

This work focuses on the atomic structure of doped $SrTiO_3(001)$ perovskite surface and the potential to modify its catalytic activity by the presence of extrinsic metals, with the main focus on cobalt. Combined STM/AFM, LEED, and XPS show a combination of cobalt clustering and dispersion within an ordered reconstruction. We will highlight how cobalt interacts with perovskite surfaces at different reducing conditions and explain the various phases of the supported cobalt as a function of temperature.

The work was supported by projects MSMT LL2324, GACR 20-21727X, and GAUK 10/252122. The work was supported by projects GAUK 10/252122, GACR 20-21727X, and GAUK Primus/20/SCI/009.

O 81.8 Thu 12:15 H6

**Machine Learning Assisted Realistic Description of Mo-V Mixed Oxide Surfaces** — •Kyeonghyeon Nam, Y. Song, L. Masliuk, T. Lunkenbein, A. Trunschke, K. Reuter, and C. Scheurer — Fritz-Haber-Institut der MPG, Berlin

The activity and selectivity of realistic heterogeneous catalysts can be noticeably altered by subtle changes in factors such as bulk composition, dopants, defects, and reaction conditions. These effects are intricately interrelated. To systematically unravel them, we aim to understand their impact on the evolution of catalyst surfaces. Specifically, we focus on the M1 structural modification of (Mo,V)$O_x$ and (Mo,V,Te,Nb)$O_x$ as selective catalysts for the oxidative dehydrogenation of ethane to ethylene.

The large primitive cell of the M1 catalyst poses challenges for a detailed study of its surface terminations using conventional first-principles calculations. To overcome this, we trained machine learning interatomic potentials (MLIPs) using a staged training method from motifs to surfaces. By combining density-functional tight-binding (DFTB) calculations with simulations employing MLIPs, such as molecular dynamics and *ab initio* thermodynamics (AITD), we elucidated the influence of niobium and tellurium doping on enhanced surface structure stability and catalytic activity during the thermal activation. This was supported by experimental *quasi-operando* scanning transmission electron microscopy (STEM) images.

## O 82: Plasmonics and Nanooptics: Fabrication, Characterization and Applications II

Time: Thursday 10:30–12:30 Location: H8

O 82.1 Thu 10:30 H8

**Femtosecond Direct Laser Writing of Conductive and Electrically Switchable PEDOT:PSS Optical Nanostructures** — •Dominik Ludescher[1], Pavel Ruchka[1], Leander Siegle[1], Yanzhe Huang[2], Philipp Flad[1], Monika Ubl[1], Sabine Ludwigs[2], Mario Hentschel[1], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]IPOC - Functional Polymers, Institute of Polymer Chemistry, University of Stuttgart, Germany

Conducting polymers, exemplified by PEDOT:PSS, exhibit distinctive electronic and polymeric attributes. When subjected to CMOS-compatible voltages (-3 V and +2 V), PEDOT:PSS transitions between insulating and metallic states via an intrinsic electrochemical redox reaction. Consequently, this conducting polymer is suited perfectly for AR/VR applications, advanced display technologies, dynamic sensors, and integration with printed optics. The latter application requires a robust foundation in fabrication and the ability to combine 3D printed optics with switchable materials to open the route to dynamic miniaturized optics. We present an alternative fabrication method based on the photon-induced solubility modulation that combines conventional, static photopolymer structures (IP-S) with the dynamic behavior of PEDOT:PSS. Additionally, we demonstrate that the electrical, optical, and dynamic material properties remain even after structuring based on direct laser writing, present the resolution limit at 400 nm structure width, and investigate the switching speed and sample longevity.

O 82.2 Thu 10:45 H8

**Revolutionizing OLED Performance and Efficiency with Core-Shell Nanoparticles in HTL and Carbon Dots in ETL Layers** — •Zoi Georgiopoulou[1,2], Apostolis Verykios[1], Theodoros Triadis[1], and Maria Vasilopoulou[1] — [1]Institute of Nanoscience and Nanotechnology, National Center for Scientific Research *Demokritos* — [2]Solid State Physics Section, Department of Physics, National and Kapodistrian University of Athens

The development of efficient organic light-emitting diodes (OLEDs) is essential for advancing modern displays and flexible electronics. This presentation explores two methodologies to enhance OLED performance through innovative material integration. The first involves incorporating core-shell nanoparticles into the hole transport layer (HTL). Metal nanoparticles (M-NPs) are encapsulated in a tungsten polyoxometalate (POM) compound and embedded in the PEDOT:PSS layer, leveraging the Localized Surface Plasmon Resonance (LSPR) effect. Analyses, including UV-Vis spectroscopy, atomic force microscopy, and electrical measurements, reveal enhanced optoelectronic properties with POM-M-NP integration. The second approach enhances OLED efficiency by combining carbon dots and a porphyrin layer in the electron transport layer (ETL). Carbon dots improve electron mobility and reduce recombination losses, while the porphyrin layer facilitates charge injection and blocks backflow. This synergy optimizes charge balance, lowers operating voltage, and improves luminous efficiency. These strategies underscore the importance of advanced material engineering in OLED development

O 82.3 Thu 11:00 H8

**Engineered disorder metasurfaces for near-field light shaping** — •Luca Schmid[1], Julian Schwab[1], Chi Li[2], Stefan Maier[2], Harald Giessen[1], Haoran Ren[2], and Mario Hentschel[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]School of Physics and Astronomy, Monash University, Clayton, Victoria, Australia

Plasmonic and dielectric nanophotonic building blocks allow for shaping the flow of light at boundaries and interfaces. They have opened the field of metasurfaces, which until now mostly allow for the creation of nearly arbitrary far-field intensity distributions in the far field. Drawing inspiration from this concept, we introduce metasurfaces for near-field light shaping. Desired near-field intensity distributions can be created by engineering the distribution of individual scatterers on metallic surfaces and hence the interference of the individually launched surface plasmons. Using this ansatz, we demonstrate engineered-disorder metasurfaces which enable to direct, focus, and demultiplex incident light. We implement these structures by a peel-off process from molds, which results in ultra-smooth metallic surfaces, maximizing the plasmon propagation length. Far-field measurements based on a k-space spectroscopy setup allow us to image the local near-field and show excellent agreement with modelling and simulation. We envision that the creation of nearly arbitrary near-field distributions will enable nanoscale routing and sorting of light based on polarization, orbital angular momentum, and wavelength, as well as help realize novel coupling schemes to emitters and nanoscale systems.

O 82.4 Thu 11:15 H8

**Strong polarization-tuned optical nonlinearity via femtosecond-laser plasmonic nanolithography in lithium niobate** — •Han Zhu[1,2], Shengqiang Zhou[1], and Feng Chen[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Shandong University, Jinan 250100, China

Despite the advantages of lithium niobate (LN)-based photonic integration platforms in various applications, the inherently weak third-order nonlinear optical response of conventional materials limits the miniaturization and energy efficiency of nonlinear optical devices in compact optical systems. Localized surface plasmons (LSPs) provide a promising solution to this miniaturization challenge by confining and enhancing light fields at deep subwavelength scales. However, due to nanofabrication limitations, strongly coupled single-crystal LN-LSP structures have yet to be realized. Here, we demonstrate Au nanorod-LN hybrid plasmonic structures assembled via plasmonic nanolithography. By leveraging plasmon-mediated energy deposition and photon momentum transfer under femtosecond laser irradiation, the nanoparticles within the single-crystalline region are formed from implanted elements. With plasmons excited in distinct axial directions, the resulting nanorod-LN hybrid plasmonic material exhibits polarization-dependent nonlinearity, with the nonlinear absorption coefficient for long-axis polarized light augmented by five orders of magnitude compared to the pure LN. Utilizing this feature, we develop a Q-switched laser exhibiting pronounced polarization-dependent behavior.

O 82.5 Thu 11:30 H8

**Nonlocal Substrate Influence on the Plasmon of a Supported Silver Nanoparticle** — Kevin Oldenburg, Karl-Heinz Meiwes-Broer, and •Ingo Barke — ELMI-MV, Department *Life, Light & Matter*, and Institute of Physics, University of Rostock

The effect of a substrate on a particle plasmon (Localized Surface Plasmon Resonance, LSPR) is often considered to be of local nature, where the substrate primarily affects the plasmon at short distances [1]. Here we present spatially resolved plasmon excitation probabilities of a single 11 nm silver nanoparticle deposited from the gas phase onto a narrow rim of a carbon substrate ("cliffhanger"), thus providing a cross-sectional view. We employ electron energy loss spectroscopy (EELS) with a scanning transmission electron microscope (STEM) where we find the strongest substrate effect, i.e., the largest red shift, when the plasmon is excited farthest away. As will be discussed, this non-local substrate influence is a consequence of the simplicity and size of the system. These results are corroborated by simulations based on the boundary element method (BEM), which also help extract the full mode structure from the experimental data. Furthermore, we observe pronounced symmetry breaking, lifting the threefold degeneracy of the dominating dipole modes, potentially resolving long-standing discrepancies in the literature regarding plasmon energies of silver clusters in this size regime [2].

[1] S. Mazzucco, et al., Nano Letters 12, 1288 (2012).

[2] H. Haberland, Nature (2013), 494 E1-E2; A. Campos et al., Nature Physics (2019), 15, 275

O 82.6 Thu 11:45 H8

**Dynamic beam switching using individually adressable plasmonic gratings made from switchable metallic polymer in planar technology** — •Jonas Herbig, Dominik Ludescher, Monika Ubl, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

The ability to steer light in an optical system is vital for light detection and ranging (LiDAR) applications as required for autonomous driving and technology based on artificial intelligence (AI). One relevant drawback of conventional LiDAR platforms is their large size, making them unsuitable for integration into compact devices. Here, we demonstrate a compact and programmable electrode nanopattern utilizing the structuring of indium tin oxide (ITO) layer in conjunction with the conducting polymer poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS). This structure demonstrates the individual addressability of multiple subgratings, enabling switching between different superlattice periods with CMOS-compatible voltages, resulting in multiple diffraction angles of up to 26° at a wavelength of 2150 nm. This work lays the foundation for adaptive optics as well as single addressable pixels necessary for advanced display systems and other active devices, such as spatial amplitude and phase modulators exceeding 1000 l/mm.

O 82.7 Thu 12:00 H8

**Disorder-driven localization of surface plasmon resonances in disordered assemblies of gold nanoparticles** — •Kristina Weinel[1,2,3], Johannes Schultz[1], Mohammed Fayis Kalady[1], Daniel Wolf[1], Leonardo Agudo Jácome[3], and Axel Lubk[1,2] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Dresden, Germany — [2]Technical University Dresden (TUD) Dresden, Dresden, Germany — [3]Federal Institute of Materials Research and Testing (BAM), Berlin, Germany

The general wave phenomenon of Anderson localization, which is the absence of diffusion of waves in disordered systems, is studied for surface plasmon waves in two-dimensional disordered systems. To that end disordered assemblies of plasmonic gold nanoparticles (NPs) on an insulating silicon oxide substrate were synthesized by a newly developed synthesis method where an electron beam in a scanning electron microscope is used to heat a gold microparticle precursor until evaporation and deposition of the gold atoms on the substrate forming NPs of varying sizes. To reveal the surface plasmons and their localization behavior, electron energy loss spectroscopy in the transmission electron microscope is applied and compared with self-consistent dipole model simulations. Disorder-driven spatial and spectral localization of the hybridized localized surface plasmon modes was found experimentally and via simulation. Moreover, the localization exhibits a characteristic thickness dependency determining the localization length dependency on the plasmon energy.

O 82.8 Thu 12:15 H8

**Nanophotonics of ultra-thin gold flakes** — •Gayathri Haridas, Farid Aghashirinov, Julian Schwab, Bettina Frank, and Harald Giessen — 4-th Physics Institute, University of Stuttgart, Germany

In our work, we focus on fabricating ultrathin single-crystalline gold platelets using an electrochemical synthesis approach. This process involves the reduction of gold atoms from the electrode surface to form gold ions, which then nucleate as seeds and grow into well-defined crystalline platelets. By systematically adjusting and controlling the growth parameters, we aim to optimize the synthesis conditions to achieve reproducible and stable fabrication of platelets with precise control over their lateral size and thickness. The characterization of the synthesized platelets is carried out using spectroscopic techniques such as Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM), to understand the surface morphologies and height profiles of the crystals.

The primary objective is to reduce the thickness of platelets to the single-digit nanometer scale while maintaining their lateral sizes. At this regime, the gold platelets exhibit unique optical and electrical properties that are highly sensitive to their size. This arises from the quantization of electronic states. We are particularly interested in probing these quantum effects, which can give rise to further research in the field of quantum plasmonics and thereby establishing gold as a suitable platform for it.

## O 83: 2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)

Time: Thursday 10:30–12:30 Location: H11

O 83.1 Thu 10:30 H11

**Charge ordered phases in the hole-doped triangular Mott insulator 4*Hb*-TaS$_2$** — •Byeongin Lee[1], Junho Bang[1], Hyungryul Yang[1], Sunghun Kim[2], Dirk Wulferding[3], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics, Ajou University, Suwon 16499, Republic of Korea — [3]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Republic of Korea

4*Hb*-TaS$_2$ has a unique layered structure, featuring a heterojunction between a 2D triangular Mott insulator and a charge density wave metal. Since a frustrated spin state in the correlated insulating layer is susceptible to charge ordering with carrier doping, it is required to investigate the charge distribution driven by interlayer charge transfer to understand its various phases. In this study, we utilize scanning tunneling microscopy and spectroscopy (STM/S) to examine the charge-ordered phases of 1*T*-TaS$_2$ layers within 4*Hb*-TaS$_2$, explicitly focusing on the non-half-filled regime. Our STS findings reveal an energy gap that exhibits an out-of-phase relation of the charge density. We attribute the emergence of the charge-ordered insulating phase in a doped triangular Mott insulator to the interplay between on-site and nonlocal Coulomb repulsion.

O 83.2 Thu 10:45 H11

**Superlattice engineering in graphene and 1T-NbSe$_2$ heterostructures** — •Keda Jin[1,2], Lennart Klebl[3], Junting Zhao[1,2], Tobias Wichmann[1,5], F. Stefan Tautz[1,5], Felix Lüpke[1], Dante Kennes[4], Jose Martinez-Castro[1,2], and Markus Ternes[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany — [3]I. Institute for Theoretical Physics, Universität Hamburg, 22607 Hamburg, Germany — [4]Institut für Theorie der statistischen Physik, RWTH Aachen, 52074 Aachen — [5]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany

Superlattice engineering has become a major branch of condensed matter research, not at least due to the variety of exotic states observed twisted in van der Waals heterostructures. We here present a new method to periodically modulate graphene by stacking it on 1T/2H-NbSe$_2$. By tuning the twist angle, we realized two near-commensurate superlattices: $\sqrt{3} \times \sqrt{3}$ and $2 \times 2$ aligned with the charge density wave (CDW) of 1T-NbSe$_2$. Using scanning tunnelling microscopy, we visualized local stacking configurations for these two superlattices. We applied a newly developed symmetry analysis method to track rotational symmetry breaking as a function of bias. In the $2 \times 2$ superlattice, $C_3$ rotational symmetry was preserved. However, in the $\sqrt{3} \times \sqrt{3}$, a strong strip phase occurs. This symmetry breaking is explained by our tight-binding model. Our findings highlight a mechanism for superlattice-induced symmetry breaking that hints towards exotic states of matter.

O 83.3 Thu 11:00 H11

**Influence of Edge Termination on the Electronic Structure of Single Layer MoS$_2$ on Graphene/Ir(111)** — •Alice Bremerich[1], Marco Thaler[2], Thais Chagas[1], Borna Pielic[1], Laerte Patera[2], and Carsten Busse[1] — [1]Universität Siegen, Deutschland — [2]Universität Innsbruck, Österreich

MoS$_2$ is the prototypical semiconducting single-layer transition-metal dichalcogenide (TMDC). It exhibits a metallic edge state that induces partial charge accumulation at its edges, resulting in band bending effects. This 1D state acts as a barrier to electron transport across the edge and contributes significantly to quantum confinement effects in TMDC islands. In this study, we tune the edge state and the associated band bending by altering the edge termination of MoS$_2$/gr/Ir(111) and investigate the resulting changes in the electronic structure by Scanning Tunneling Microscopy and Spectroscopy (STM and STS) at 8 K.

Quasi-freestanding $MoS_2$ is grown on gr/Ir(111) by Molecular Beam Epitaxy (MBE). We prepare hexagonal islands that exhibit two geometrically different edge types (Mo- and S-type). We vary the chemical potential of sulfur and thereby modify the chemical environment of the boundaries. The partial charge at the perimeter depends on edge type as well as edge chemistry. In consequence, also the upward bending of both valence and conduction band shows distinct variations.

O 83.4 Thu 11:15 H11

**magnetic-field-induced dimensionality transition of charge density waves in strained 2H-NbSe2** — •Ryo Ichikawa[1], Yukiko Takahashi[2], Eiichi Inami[3], and Toyo Kazu Yamada[1,4] — [1]Department of Material Science, Chiba University — [2]National Institute for Material Science, Tsukuba — [3]School of system Engineering, Kochi University of Technology — [4]Molecular Chirality Research center, Chiba University

Layered transition metal dichalcogenides (TMDs) exhibit various correlated phases, including charge density waves (CDW), superconductivity, and magnetic orders. Bulk 2H-NbSe2 (2H niobium diselenide) is one of the most extensively studied TMDs, showing a triangular (3Q) incommensurate CDW with a 3a period in real space (3 * 3, TCDW ~ 33 K). Electric and magnetic fields have been used to manipulate spatial or time inversion symmetry, while the CDW in 2H-NbSe2 remains robust even under large magnetic fields on the order of tens of Tesla. However, magnetic-field-sensitive CDWs have been reported in few-layer NbSe2, where a weak magnetic field of approximately 30 mT can switch the electronic phase within the thin film, resulting in a supercurrent diode effect. This study investigates the strained 2H-NbSe2 exhibiting the 2*2 CDW phase. We utilize low-temperature (4.3 K) scanning tunneling microscopy and spectroscopy (STM/STS) in ultra-high vacuum (UHV). STS maps reveal the coherence of the 2*2 CDW patterns. However, applying an out-of-plane magnetic field induces a dramatic transformation akin to that observed in 1T-NbSe2, shifting the metallic 2D CDW pattern to a 1D CDW pattern.

O 83.5 Thu 11:30 H11

**Ultrafast phonons dynamics of monolayer transition metal dichalcogenides** — •yiming pan and fabio caruso — Kiel University, Germany

Valley degrees of freedom in transition-metal dichalcogenides influence thoroughly electron-phonon coupling and its nonequilibrium dynamics. Here we present a time-resolved ab-initio study of the ultrafast dynamics of chiral phonons following carrier excitation with circularly-polarized light. By investigating the valley depolarization dynamics of monolayer $MoS_2$ and $WS_2$, we find that a population imbalance of carriers distributed at K and K′ can lead to valley polarized phonons persisting beyond 10 ps, and characterized by a distinctive chirality [1]. Additionally, we find that strain can be exploited as a tool to control the phonon emission and the relaxation channels of hot carriers [2]. Finally, we briefly discuss available opportunities for experimental detection of these phenomena

[1] Y. Pan and F. Caruso, Nano Lett. 23, 7463 (2023)
[2] Y. Pan and F. Caruso, npj 2D Mater. Appl. 8, 42 (2024)

O 83.6 Thu 11:45 H11

**Probing Excitonic Properties and Structural Effects in $WS_2$-Graphene Heterostructures Using EELS and DFT-BSE Modeling** — •Max Bergmann, Jürgen Belz, Oliver Massmeyer, Robin Günkel, Badrosadat Ojaghi Dogahe, Andreas Beyer, Stefan Wippermann, and Kerstin Volz — Department of Physics, Philipps-Universität Marburg, Germany

This study investigates the excitonic properties of $WS_2$ epitaxially grown on graphene by metal-organic chemical vapor deposition. We focus on understanding the effects of structural changes, such as variations in the number of $WS_2$ layers. Using monochromatic electron energy loss spectroscopy (EELS) in a scanning transmission electron microscope (STEM), we observe in the monolayer region of $WS_2$ an excitonic spectrum with excitonic peaks at 2.0 eV and 2.4 eV, as well as additional spectral features at higher energies. Measurements in the bilayer region show a small redshift of these features due to the additional layer. Complementary density functional theory and Bethe-Salpeter calculations show that this redshift in the K-valley excitons is due to both a change in quantum confinement and a change in the $WS_2$ lattice constant, with the latter being the dominant effect. Using STEM, this lattice distortion can be attributed to the heteroepitaxial alignment of the lower $WS_2$ layer to the graphene substrate, while the upper layer is relaxed. This study provides valuable insights into the relationship between atomic structure and optical properties in complex material systems, providing essential knowledge for the design and optimization of 2D heterostructures for advanced device applications.

O 83.7 Thu 12:00 H11

**Optical excitations in 2H-$MoS_2$ bilayers under pressure** — •Jan-Hauke Graalmann[1], Paul Steeger[2], Rudolf Bratschitsch[2], and Michael Rohlfing[1] — [1]University of Münster, Institute of Solid State Theory, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]University of Münster, Institute of Physics and Center for Nanotechnology, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Theoretical and experimental investigations have shown several changes in the optical spectrum of the 2H-$MoS_2$ bilayer under pressure [1].

By using density functional theory (DFT) and many-body perturbation theory in combination with linear elasticity, our computational investigations show an effective shift of the A exciton under pressure. It is strongly connected to the behavior of the direct band gap at the K point, which shifts in energy under pressure. The direction of this shift depends on the stress condition. While a hydrostatic pressure leads to a blueshift, a suppression of the in-plane contraction, as it appears in diamond anvil cell-experiments due to the interaction between the sample and the substrate, shows a redshift.

Moreover, we observe a similar behavior for the interlayer exciton, whereas the shift rate is smaller than that of the A exciton, which results in a decreasing A-IL splitting for an increasing pressure.

[1] P. Steeger, J. Graalmann et al., Nano Lett., 23, (2023)

O 83.8 Thu 12:15 H11

**Visualizing and controlling charge states of metal nanoislands on a two dimensional semiconductor** — •Junho Bang[1], Byeongin Lee[1], Jian-Feng Ge[2], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul, Korea — [2]Department of Topological Quantum Chemistry, Max Planck Institute for Chemical Physics of Solids, München ,Germany

Nanoscale objects show unique electronic behaviors when weakly coupled to electrodes. Coulomb blockade (CB) can occur in such systems, where the repulsive Coulomb interaction between electrons prevents additional electrons from entering the quantum dots, hindering their flow. Single electron tunneling occurs by these correlated electron transports, leading to the discrete charge states of objects in double barrier tunneling junctions. Despite enormous progress, challenges remain in precisely controlling the interplay between objects' charge states and tunneling dynamics under varying conditions. Here, we visualize the charge states and their spatial variation on the random array of the indium islands on two-dimensional semiconductor black phosphorus using scanning tunneling microscopy and spectroscopy. Our spatially resolved tunneling spectra reveal that the junction capacitance varies across the islands. Furthermore, we find that the CB features are visible outside the islands, which is attributed to the remote gating of the islands. Our work advances the manipulation of electron transport at the nanoscale, which will be helpful in the application of nanoscale object-based single-electron devices.

# O 84: Gerhard Ertl Young Investigator Award Competition

Time: Thursday 10:30–13:00 Location: H24

O 84.1 Thu 10:30 H24

**CO cryo-sorption on a FeNC catalyst as a spectroscopic probe of the active site density** — •Benedikt P. Klein[1,3], Beomgyun Jeong[1], Hafiz Ghulam Abbas[2], Geunsu Bae[2], Adith R. Velmurugan[2], Chang Hyuck Choi[4], Geonhwa Kim[5], Dongwoo Kim[5], Ki-jeong Kim[5], Byeong Jun Cha[6], Young Dok Kim[6], Frederic Jaouen[7], Reinhard J. Maurer[3], and Stefan Ringe[2] — [1]Korea Basic Science Institute, Daejeon, ROK — [2]Korea University, Seoul, ROK — [3]University of Warwick, Coventry, UK — [4]POSTECH, Pohang, ROK — [5]PAL, Pohang, ROK — [6]Sungkyukwan University, Suwon, ROK — [7]University of Montpellier, France

To quantify the number of active sites in a catalyst is a crucial necessity for the evaluation of its performance. A possible quantification approach is the adsorption of a gas molecule to the catalytically active sites as a probe. If the adsorbed molecules can be reliably detected, their surface density can be determined by using spectroscopic techniques and the active site density of the catalyst can be obtained. For this approach it is necessary to identify the probe molecules according to their spectroscopic features, a task much helped by the computational simulation of spectra. In this the NAP-XPS and NAP-NEXAFS study, we present direct spectroscopic evidence for the adsorption of CO on an iron-nitrogen-carbon (FeNC) catalyst. The well defined spectroscopic features enable us to determine the active site density using by experimental data combined with state-of-the-art DFT based spectroscopy simulation.

O 84.2 Thu 11:00 H24

**Nano-optical imaging of grating-coupled waveguide modes in 3R-MoS$_2$** — •Fabian Mooshammer[1], Xinyi Xu[2], Chiara Trovatello[2], P. James Schuck[2], and D. N. Basov[3] — [1]Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany — [2]Department of Mechanical Engineering, Columbia University, New York, USA — [3]Department of Physics, Columbia University, New York, USA

Waveguide modes in thin slabs of van der Waals crystals serve as reliable probes of the anisotropic dielectric response of the material and also hold great potential for the implementation of on-chip optical elements. Here, we show that near-field imaging can resolve the propagation patterns of waveguide modes, which encode the birefringence of transition metal dichalcogenides. We use a laser patterning procedure to write grating structures into 3R-MoS$_2$ crystals with grooves as sharp as 250 nm. Spatial maps of the scattered electric field in the vicinity of the gratings reveal a directional, polarization-splitting outcoupling of waveguide modes, which is in line with finite element simulations. Experiments over a range of near-infrared photon energies provide key parameters for waveguide second-harmonic generation. The latter is finally demonstrated by grating-coupling femtosecond pulses into the slabs. In the future, nano-optical imaging may be used to directly capture the frequency conversion process during the propagation of the modes. Our work demonstrates the feasibility of compact frequency converters and examines the tunings knobs that enable optimized coupling into layered waveguides.

O 84.3 Thu 11:30 H24

**Imaging Infrared Materials Excitations with Sum-Frequency Spectro-Microscopy** — •Niclas S. Mueller[1], Alexander Fellows[1], Richarda Niemann[1,2], Andrew E. Naclerio[2], Ryan A. Kowalski[2], Ben John[1], Katayoun Gharagozloo-Hubmann[3], Soeren Wasserroth[1], Guanyu Lu[2,4], Joshua D. Caldwell[2], Piran R. Kidambi[2], Martin Wolf[1], Martin Thaemer[1], and Alexander Paarmann[1] — [1]Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany — [2]Vanderbilt University, Nashville, TN, USA — [3]Freie Universitaet Berlin, Berlin, Germany — [4]Northwestern University, Evanston, IL, USA

Nonlinear optical microscopy and spectroscopy are powerful tools to characterize interfaces and lower-dimensional materials. Here, I show two examples how we use infrared + visible sum-frequency generation (SFG) to image mid-infrared materials excitations with wide-field optical microscopy. The techniques provide combined spatial and spectral information, with sub-diffractional spatial resolution. 1. We visualize the propagation of infrared phonon polaritons in a metasurface of silicon carbide [1]. Through a combination of microscopy and spectroscopy, we observe the hybridization and strong coupling of propagating and localized polaritons, as well as the activation of edge states. 2. We visualize monolayers of hexagonal boron nitride, which are usually optically invisible. Resonant infrared excitation of phonons and heterodyne sum-frequency imaging enable us to image, both, the local topography and crystal orientation with unprecedented detail.

[1] Niemann, Mueller et al. Advanced Materials 36, 2312507 (2024)

O 84.4 Thu 12:00 H24

**Towards Understanding Surface Restructuring: Automatic Process Exploration and Local Environment Analysis** — •Patricia Poths, King Chun Lai, Francesco Cannizzaro, Christoph Scheurer, Sebastian Matera, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

The formation of surface oxides on the Pd(100) surface is a prototypical example of catalyst surface restructuring under *operando* conditions. Despite extensive investigation of this process, its mechanism and corresponding time scales remain unknown. By combining a Machine-Learned Interatomic Potential with our newly-developed Automatic Process Explorer (APE) [1], we study the O-induced restructuring of the Pd(410) vicinal surface as an example for step-edge initiation of oxide formation. We identify ∼3,000 unique elementary processes. Taking first steps towards a comprehensive mechanism, we analyze this rich library of processes utilizing a fuzzy classification methodology [2]. Many identified pathways involve non-intuitive complex collective motion of several atoms. These pathways can explain experimentally-observed restructuring, such as step bunching or microfaceting. Furthermore, the time scales of the majority of restructuring pathways are comparable to those of catalytic processes, implying significant coupling between surface restructuring and catalysis [3].

[1] Lai *et al.*, ChemRxiv, DOI:10.26434/chemrxiv-2024-jbzr7 .

[2] Lai *et al.*, J. Chem. Phys. **159**, 024129 (2023).

[3] Poths *et al.*, ChemRxiv, DOI:10.26434/chemrxiv-2024-36l28 .

O 84.5 Thu 12:30 H24

**band engineering via metal substitution in porphyrin-graphene hybrid systems** — •feifei xiang[1], yanwei gu[2], amogh kinikar[1], nicolò bassi[1], andres ortega-guerrero[1], carlo a. pignedoli[1], giovanni bottari[3], tomás torres[3], klaus müllen[2], pascal ruffieux[1], and roman fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — [2]Synthetic Chemistry, Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [3]Departamento de Química Orgánica Universidad Autónoma de Madrid Madrid 28049, Spain

Graphene and its derivatives serve as a versatile platform for finely tuning physical properties across a wide range. Expanding the potential applications of graphene to optoelectronics and gas sensing has driven the development of new materials including hybrid molecular systems that integrate porphyrins with graphene. On-surface synthesis provides a viable approach to achieving such well-defined hybrid structures. Here, we present the synthesis and characterization of porphyrin-graphene hybrid systems (chemrxiv-2024-z9rgh), in which the porphyrin units feature varying metal substitutions. The strong electronic coupling between porphyrin and tailored graphene nanostructures enables the metal center to play a significant role in modulating the band structure through charge doping, and to generate new hybrid states arising from d-$\pi$ interactions, which allows long range spin coupling between magnetic metal centers. Such robust hybrid molecular systems hold promise in applications in p-n heterojunctions and paves the way towards achieving coherent control of spin chains.

# O 85: New Methods: Theory

Time: Thursday 10:30–12:45 Location: H25

O 85.1 Thu 10:30 H25

**Quantifying the conductance of molecular structural variables using machine learning** — •Hector Vazquez — Inst. of Physics, Czech Academy of Sciences

In single molecule electronics, where individual molecules are placed between two nanoscale electrodes, conductance depends critically on the geometry at the junction. Atomistic simulations using DFT-NEGF are ideally suited to address this, but their computational cost restricts their use to only few junction geometries. In experiments, however, molecular geometry is thought to change significantly since measurements are often carried out at room temperature.

Here we use an approximate method to calculate molecular conductance within DFT for thousands of geometries [1]. The method uses small Au-molecule-Au clusters and is thus computationally very efficient, yet reproduces DFT-NEGF conductance well. Combined with MD simulations of the junction, we compute for thousands of geometries the variation in conductance arising from thermally-induced conformational changes in the molecule.

We use machine-learning methods to identify which of the molecular structural parameters, all of which are changing continuously and simultaneously during the MD simulations, have a greater impact in conductance. This elucidates how molecular conformational changes contribute to the width of the conductance signal in single molecule junctions.

[1] H. Vazquez, J. Phys. Chem. Lett. 13 9326 (2022)

O 85.2 Thu 10:45 H25

**Efficient implementation of charge-equilibration schemes for fourth-generation machine learning potentials** — •Moritz R. Schäfer[1,2], Moritz Gubler[3], Stefan Goedecker[3], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Department of Physics, University of Basel, Switzerland

Fourth-generation high-dimensional neural network potentials (4G-HDNNPs) are a modern technique to compute energies and forces with close to ab initio accuracy for conducting extensive molecular dynamics simulations of complex systems. They are based on global information and include long-range charge transfer, electrostatics and atomic energies to describe the interactions in a system. A central component of 4G-HDNNPs is a charge equilibration ($Q_{eq}$) step, which due to its non-local nature dominates the computational costs. Here, we discuss efficient implementation strategies, and show their performance on selected benchmark systems.

O 85.3 Thu 11:00 H25

**Real-time Bethe-Salpeter Equation for optical properties of molecules – Implementation and benchmark calculations** — •Štěpán Marek, Maximilian Graml, and Jan Wilhelm — Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, Regensburg, Germany

We present an implementation of a real-time version of the Bethe-Salpeter equation (RT-BSE) in CP2K, offering new capabilities for investigating electron dynamics in molecules under laser excitation. The RT-BSE implementation is tested on Thiel's molecular benchmark set - a set of organic molecules of various types. We evaluate the accuracy and performance of the RT-BSE approach for the determination of absorption spectra of molecules, with respect to the Casida-BSE approach. We discuss the scaling of the method to show its potential for studying optical properties of large molecules and complex materials.

O 85.4 Thu 11:15 H25

**Extension of FLAPW method `FLEUR` to phonon calculations of polar solids using DFPT** — •Friedrich Hanrath[1,2], Thomas Bornhake[1,2], Gregor Michalicek[1], Daniel Wortmann[1], Gustav Bihlmayer[1], and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Physics Department, RWTH Aachen University, Aachen, Germany

Phonons play a pivotal role in determining important properties of solids. In polar materials, phononic vibrations are altered by the interaction of macroscopic electric fields in the limit of long wavelengths. This gives rise to the characteristic splitting of longitudinal and transversal optical phonon frequencies. Density function perturbation theory (DFPT) is a state-of-the-art approach to calculate many essential physical properties of solids from first principles. By using an ionic displacement perturbation, it has previously been employed in order to calculate phonons in the framework of the full-potential linearized augmented plane-wave method `FLEUR` [1, 2]. — In this talk, this method is extended to a macroscopic homogeneous electric field perturbation allowing the calculation of static dielectric properties, Born effective charges and hence LO-TO-splitting. We present the current results for the static dielectric tensor for various semiconductors and insulators by comparing them with experimental results.

This work was supported by the CoE-MaX (EuroHPC JU, Grant No. 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).

O 85.5 Thu 11:30 H25

**Efficient treatment of long-range electrostatics in charge equilibration approaches** — •Kamila Savvidi, Ludwig Ahrens-Iwers, and Robert Meissner — Hamburg University of Technology, Hamburg, Germany

We present a charge equilibration (QEq) method in the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) based on real-space Gaussians of width $\eta_i$ as charge densities. This implementation builds on the `ELECTRODE` package, which already supports Gaussian charge densities [1]. In addition, an efficient particle-particle particle-mesh $k$-space solver [2] is used, which significantly improves the computational performance compared to existing QEq implementations in LAMMPS. We validate our approach with the test cases of Ti/TiO$_\mathrm{x}$ and SiO$_2$ polymorphs. In the limit of very narrow Gaussians, we were able to show that our algorithm converges to EEM results for the case of Ti/TiO$_\mathrm{x}$. By fitting the Coulomb energy of two isolated Gaussian charge distributions to the repulsion between two Slater-type orbitals, optimized widths for Si and O were obtained that led to results in good agreement to previous studies using STOs instead of Gaussians.

[1] Ludwig J. V. Ahrens-Iwers, Mathijs Janssen, Shern R. Tee, Robert H. Meißner; ELECTRODE: An electrochemistry package for atomistic simulations. J. Chem. Phys. 28 August 2022; 157 (8) [2] Ahrens-Iwers LJV, Meißner RH. Constant potential simulations on a mesh. J Chem Phys. 2021 Sep 14;155(10)

O 85.6 Thu 11:45 H25

**Machine Learning for Polaronic Materials: TiO$_2$(110) at the nanoscale** — •Firat Yalcin[1], Simon Trivisonne[1], Viktor Birschitzky[1], Carla Verdi[2], and Michele Reticcioli[1,3] — [1]University of Vienna, Austria — [2]University of Queensland, Australia — [3]CNR-SPIN L'Aquila, Italy

The combination of machine learning (ML) with density functional theory accelerates material simulations, expanding both spatial and temporal scales. However, current ML methods struggle to address polaron trapping. We present a novel machine learning force field (MLFF) approach that incorporates polaron trapping descriptors, enabling large-scale studies of polaronic materials. Using TiO$_2$(110) as a case study, we reveal how Nb dopants and oxygen vacancies affect polaron configurations and drive catalytic CO adsorption. Additionally, our method captures the dynamic evolution of polarons with unprecedented statistical robustness. This work advances fundamental understanding of defect-polaron interactions while offering a fully-automated and efficient computational suite for the study of polaronic materials.

O 85.7 Thu 12:00 H25

**Uncertainty quantification for DFT calculations** — •Teitur Hansen[1], Thomas Bligaard[2], and Karsten W. Jacobsen[1] — [1]DTU Physics, Kongens Lyngby, Denmark — [2]DTU Energy, Kongens Lyngby, Denmark

Density functional theory (DFT) is widely used for understanding material properties and chemical reactions. DFT simulations use approximations which result in errors when comparing to experiments. There are errors in different types of energies, lattice constants and other properties. Quantitative uncertainty estimates would be helpful for DFT simulations to highlight which results are trustworthy. Quantifying uncertainties not only improves trust in calculations but also identifies high-uncertainty predictions that can subsequently be revisited and reanalyzed.

We propose a method to model uncertainties using a probability distribution over exchange-correlation functionals. The probability distribution is trained on experimental values of molecular atomization energies, cohesive energies of solids, reactions energies, heat of formations, and lattice constants. The optimized probability distribution is then used to define an ensemble method which can be used to estimate the bias and variance on simulated materials properties. I will demonstrate that the method gives systematic improvements in error estimates over the Bayesian error estimation class of functionals (BEEF).

The proposed method is general enough to be applied to any simulation methodology where accurate reference benchmarks exist.

O 85.8 Thu 12:15 H25

**Assessment of the Accuracy of Equation-of-motion Coupled-cluster band gaps in the Bulk Limit** — •Evgeny Moerman[1], Alejandro Gallo[2], Andreas Irmler[2], Andreas Grüneis[2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI-MPG, Berlin — [2]Institute for Theoretical Physics, TU Wien, Vienna

As a highly regarded theoretical framework in molecular quantum chemistry, coupled-cluster (CC) theory is expected to yield reliable and systematically improvable results for both ground-state and ex cited state properties of materials. One major obstacle to obtaining converged CC results for periodic solids is the often slow convergence with respect to system size. We have investigated the finite-size convergence behaviour of band gaps in equation-of-motion CC (EOM-CC) theory and revealed a direct relation to the GW approximation [1]. Based on these findings, a GW-aided scheme to reliably estimate the size-converged EOM-CC band gap has been developed and tested [2], allowing to assess the true accuracy of the widely used EOM-CCSD method in the periodic case. We find that the accuracy of EOM-CCSD band gaps sensitively depends on the magnitude of orbital relaxation effects, suggesting that such low-order truncation methods as EOM-CCSD may not be sufficiently accurate even for simple materials and that higher orders of correlations seem to be necessary. - This work received support from the European Union's Horizon 2020 research and innovation program under Grant Agreement No.740233.

[1] Moerman et al., arXiv:2409.03721 (2024)

[2] Moerman et al., to be published

O 85.9 Thu 12:30 H25

**Full periodic real-time TD-DFTB implementation for solids and low-dimensional materials** — •Carlos R. Lien-Medrano[1], Franco P. Bonafé[2], Matías Berdakín[3], Cristián G. Sánchez[4], and Michael Sentef[1,2] — [1]University of Bremen, Bremen, Germany — [2]MPSD, Hamburg, Germany — [3]Universidad Nacional de Córdoba, Córdoba, Argentina — [4]Universidad Nacioanl de Cuyo, Mendoza, Argentina

The current real-time time-dependent density functional tight-binding (TD-DFTB) dynamics implementation in the DFTB+ package [1] employs the length gauge of the electric field. In this work, we introduce an implementation of the vector potential within the velocity gauge framework. This approach enables the extension of real-time dynamics simulations to periodic systems along arbitrary spatial directions, making it applicable to photo-induced dynamical processes in bulk, low-dimensional materials, and surfaces. To demonstrate its potential, we present proof-of-concept applications, including the inhomogeneous optical absorption around the K point in graphene, light absorption in bulk materials, and prospective applications in the field of valleytronics.

[1] Hourahine, B., et al. (2020). DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. The Journal of Chemical Physics, 152(12), 124101.

## O 86: Electronic Structure of Surfaces: Spectroscopy, Surface States II

Time: Thursday 15:00–17:30 Location: H2

O 86.1 Thu 15:00 H2

**Low temperature STM/AFM detection of 2D electronic gas on reduced $SrTiO_3$ surface** — •Akash Gupta, Marcin Kisiel, Remy Pawlak, and Ernst meyer — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Perovskite such as $SrTiO_3$ ubiquitous to host various reconstruction with fine tuning of the annealing temperature. At 1050°C, in oxygen poor conditions, a $\sqrt{5}\times\sqrt{5}$ surface reconstruction is formed with oxygen vacancies. These oxygen vacancies result in compactly confined electrons as two-dimensional electron gas (2DEG) system. The 2DEG is confirmed as filled surface states in Low Temperature (4 K, UHV) Scanning Tunneling Spectroscopy (STS). Additionally, Image Potential States (IPS) emerges at lower energies than vacuum level, revealing work function, as well. The charging of this 2DEG system can be induced with capacitively coupled tip of Atomic Force Microscope, and it results in giant dissipation peaks as signature of surface charging with change in the tip-sample voltage. Furthermore, quantum capacitance is calculated as function of the gate voltage. The evolution of dissipation peaks were observed with tip-sample distance. The Force-Distance curves confirm the 2DEG charging and is used to determine the tunneling rate of the charging within 2DEG system.

O 86.2 Thu 15:15 H2

**Tunneling Spectroscopy of $RuO_2$(110): Electronic Structure, Correlation Effects and Substrate Interactions** — •Philipp Kessler, Andreas Feuerpfeil, Hendrik Hohmann, Matteo Dürrnagel, Armando Consiglio, Jonas Erhardt, Michael Sing, Ralph Claessen, Ronny Thomale, and Simon Moser — Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

The (110) surface of $RuO_2$ hosts a flat band surface state (FBSS) close to the Fermi level that is prone to Fermi surface instabilities and can be readily observed in angle resolved photoemission. A local spectroscopic investigation of this FBSS to study such instabilities is, however, still outstanding. In this talk, we present the synthesis of high quality $RuO_2$(110) surfaces, enabling systematic scanning tunneling spectroscopy (STS) measurements across wide defect free domains. We observe hints of correlation effects, manifesting in signatures of a charge density wave and a zero-bias anomaly. Furthermore, we offer preliminary evidence suggesting that the electronic structure of $RuO_2$ depends on the oxide film thickness and immediate screening environment within the substrate. These findings illuminate the interplay between the Ru metal substrate and the $RuO_2$ oxide, advancing this topical material.

O 86.3 Thu 15:30 H2

**Quasi-particle interference studies on ultra-thin films of Cu(111)** — •Jungin Yeo — Chung-Ang University, Seoul 06974, Republic of Korea

Recently, ultra-thin crystalline Cu(111) film has been successfully grown on a sapphire substrate through the atomic sputtering epitaxy (ASE). In-depth studies were conducted to explore the crystal growth mechanism and the oxidation process. Ultra-thin film without grain boundary (GB) shows hidden intrinsic nature such as transport by hole carriers. Meanwhile, twin boundaries (TB) appear inevitably during the growth even such an atomically high-quality film. As two orientations adjacent to a TB satisfy the symmetry operation exactly, TBs are expected to show different electronic properties from GBs. The unique electronic properties resulting from the two-dimensional nature and the presence of TBs are currently under investigation. For our study, we utilized scanning tunneling microscopy (STM) to examine 20 nm thick ASE-grown Cu(111) films. The STM topography revealed an atomically flat surface with an indication of twin boundaries. We performed quasi-particle interference (QPI) measurements across TBs. The surface states of Cu(111) and quantum-confined states within the film thickness were successfully resolved. By analyzing the QPI data, we were able to reconstruct the electronic dispersion near the Fermi energy, both at the surface and within the bulk of 20 nm thick. The transmission probability across TBs will be discussed.

O 86.4 Thu 15:45 H2

**Electronic structure of the correlated topological metals $CoTe_2$ and $NiTe_2$** — Abhijeet Shelke[1], Chien-Wen Chuang[2], Truc Ly Nguyen[1], Yo-Xun Chen[1], Masato Yoshimura[1], Nozomu Hiraoka[1], Satoru Hamamoto[3], Masaki Oura[3], Chia-Nung Kuo[4], Chin-Shan Lue[4], Atsushi Fujimori[5,1], and •Ashish Chainani[1] — [1]National Synchrotron Radiation Research Center, Hsinchu 300092, Taiwan — [2]Dept. of Physics, Tohoku University, Sendai 980-8578, Japan — [3]RIKEN SPring-8 Center, Hyogo 679-5148, Japan — [4]Dept. of Physics, NCKU, Tainan 70101, Taiwan — [5]Dept. of Physics, The University of Tokyo, Tokyo 113-0033, Japan

The transition-metal(TM) tellurides CoTe$_2$ and NiTe$_2$ are known to exhibit topological semi-metallic Dirac bands from ARPES studies. We carry out core level and valence band measurements using hard x-ray photoemission spectroscopy(HAXPES), x-ray absorption spectroscopy(XAS) and TM $2p-3d$ resonant photoemission spectroscopy(R-PES) to study electronic structure of CoTe$_2$ and NiTe$_2$. The R-PES spectra show clear evidence of TM LVV Auger two-hole correlation satellites. Using the Cini-Sawatzky method, we estimate an on-site Coulomb energy, $U_{dd}\sim$3 eV for Co in CoTe$_2$, and $U_{dd}\sim$4 eV for Ni in NiTe$_2$. Using these values in charge-transfer cluster model calculations, we simulate the TM $2p$ HAXPES core level and $L$-edge XAS spectra of CoTe$_2$ and NiTe$_2$. The electronic parameter analyses indicate a negative charge transfer energy $\Delta$ for both CoTe$_2$ and NiTe$_2$. The results indicate a $p$-type metal in terms of the Zaanen-Sawatzky-Allen phase diagram for CoTe$_2$ and NiTe$_2$.

O 86.5 Thu 16:00 H2

**Visualizing topological ladder in PtTe$_2$** — •Mohammed Qahosh[1], Gustav Bihlmayer[2], Jakub Schusser[3], Muthu Masilamani[3], Friedrich Reinert[3], Claus M. Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum-Jülich — [2]PGI-1/IAS-1 Forschungszentrum-Jülich — [3]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg

We have examined the topological ladder [1] and band inversions in PtTe$_2$ using spin-polarized angle-resolved photoemission (spin-ARPES) with two-dimensional momentum imaging. Examining such spin images allows in-depth insight into the topological properties, not accessible by routine methods. We mapped extended momentum-space regions and visualized distinct topological ladder states, notably a surface Dirac cone at $E_B \sim 2.3$ eV, as well as states at $E_B \sim 1.0$ eV, $E_B \sim 1.6$ eV, and near the Fermi level. By comparison to *ab initio* calculations, we demonstrate a significant correlation between the measured and the initial state spin polarization. We discuss interatomic phase shifts [2] for orbitals mixed between Pt and Te sites as well as spin-orbit scattering that leads to additional spin polarization in spin-ARPES. [1] Nature Materials 17, 21 (2018). [2] Phys. Rev. Lett. 130, 146401 (2023).

O 86.6 Thu 16:15 H2

**Origin of the Spin-Polarized Fermi Surface of a Tl Bilayer on Ag(111)** — •Sven Schemmelmann[1], Yuichiro Toichi[2], Peter Krüger[3], Kazuyuki Sakamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Applied Physics, Osaka University, Japan — [3]Institut für Festkörpertheorie, Universität Münster, Germany

ARPES measurements have shown that the Fermi surface of a Tl bilayer grown on Ag(111) exhibits two hexagonal-shaped states [1]. While the inner one is fully spin polarized, the outer one appears to be unpolarized. Spin-resolved inverse photoemission experiments of the unoccupied states reveal the origin of this peculiar behavior. We observe two downward dispersing states which are both spin split. The two spin branches of the one state are responsible for the two states observed forming the Fermi surface. Interestingly, the spin up branch coincides with the spin down branch of the other downward dispersing state. This is the reason why this state appears to be unpolarized.

[1] T. Kobayashi *et al.*, Nano Lett. **23**, 7675 (2023)

O 86.7 Thu 16:30 H2

**Analyzing excitonic contributions to reflection anisotropy spectra** — •Max Grossmann[1], Kai Daniel Hanke[2], Chris Yannic Bohlemann[2], Thomas Hannappel[2], Wolf Gero Schmidt[3], and Erich Runge[1] — [1]Theoretical Physics I, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Fundamentals of Energy Materials, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [3]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

Reflection anisotropy spectroscopy (RAS) is a powerful optical tool for probing semiconductor surfaces. However, the interpretation of RA spectra is challenging due to the complex interplay of features caused by surface states and so-called surface-induced bulk anisotropy, as well as the significant influence of excitonic effects. Overcoming these challenges requires a close collaboration between experiment and theory. In this work, we combine high-quality low-temperature RAS measurements with state-of-the-art *ab initio* calculations in the framework of many-body perturbation theory to study the RAS of arsenic-terminated Si(100) surfaces. The excitonic contributions to the RAS are studied in detail through a thorough analysis of the results from a solution of the Bethe-Salpeter equation. Our approach aims to combine experimental observations with theoretical insights to decipher the complex effects that shape RAS spectra and to advance the understanding of the optical properties of semiconductor surfaces.

O 86.8 Thu 16:45 H2

**Composition and band gap of aluminum alloyed beta-gallium oxide determined by XPS** — •Lukas Schewe[1], Jana Rehm[2], Ming-Chao Kao[3], Vedran Vonk[3], Zbigniew Galazka[2], Saud Bin Anooz[2], Andreas Popp[2], and Jan Ingo Flege[1] — [1]Fachgebiet Angewandte Physik und Halbleiterspektroskopie, BTU Cottbus-Senftenberg — [2]Leibnitz-Institut für Kristallzüchtung, Berlin — [3]CXNS-Center for X-ray and Nano Science, DESY Hamburg

Beta-phase gallium oxide is a wide-gap semiconductor with a band gap of 4.85eV and promising prospects in high-power electronics. The electric breakdown field can be increased by alloying the oxide with aluminum, further enhancing its properties.

The present work discusses structural and electronic properties of $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ thin films and bulk crystals with Al content of up to 33 %. Their Al content was determined by X-ray photo-electron spectroscopy (XPS) and compared to the values estimated from X-ray diffraction (XRD) and inductively coupled plasma optical emission spectroscopy (ICP-OES). Additionally, the thin films have been investigated by XPS depth profiling, i.e., XPS combined by sequential Ar$^+$ sputtering, revealing lower aluminum content at the sample surface, which points to possible surface segregation of gallium during annealing. Furthermore, the band gap was determined by electron loss spectra from XPS and optical absorbance measurements and correlated to the Al content estimated for both thin films and bulk crystals.

O 86.9 Thu 17:00 H2

**Higher-order van Hove singularities in Kagome metal RbV$_3$Sb$_5$** — •Gahee Lee — Department of Physics, Chung-Ang University, Seoul 06974, Republic of Korea

The divergence of the density of states (DOS) near the Fermi energy is crucial for enhancing electron correlations. Van Hove singularities (vHS) commonly cause this DOS divergence, with their properties determined by the dimensionality of electron dispersion. The atomic arrangement on the surface of layered materials can influence the effective dimensionality of electron dispersion, thereby shaping the characteristics of vHS. In V-based Kagome metals RbV$_3$Sb$_5$ (A = K, Rb, and Cs), the saddle-shaped dispersion results in two-dimensional vHS. Interestingly, the surface arrangement of atoms in a Kagome lattice can modify the effective dimensionality of electron dispersion, affecting the strength of electron correlations. In this study, we present a novel approach to enhancing electron correlation by arranging the surface Rb atoms. The resulting higher-order vHS significantly enhances the divergence of DOS and strengthens charge density waves in V-based Kagome metals.

O 86.10 Thu 17:15 H2

**Single Hemisphere & Time-of-Flight Hybrid Photoelectron Momentum Microscopy** — •Olena Tkach[1], Matthias Schmitt[2,3], Deepnarayan Biswas[2], Olena Fedchenko[1], Jieyi Liu[2], Hans-Joachim Elmers[1], Michael Sing[3], Ralph Claessen[3], Tien-Lin Lee[2], and Gerd Schönhense[1] — [1]JGU Mainz, Germany — [2]DIAMOND, Didcot, United Kingdom — [3]Universität Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat, Germany

The 2ns pulse period of the photon beams from most synchrotrons is too short for pure time-of-flight (ToF) photoelectron spectroscopy. With the use of a hemispherical analyzer (HSA) as a pre-filter, ToF momentum microscopy becomes possible at such high pulse rates. The first hemisphere & ToF hybrid MM is operated at the soft X-ray branch (photon energies from 105 eV to 2 keV) of beamline I09 at DIAMOND. The HSA reduces the transmitted energy band to typically 0.5 eV, which is then dispersed by ToF recording. In the first experiments the total efficiency gain when switching from the standard 2D $(k_x, k_y)$ to the 3D $(k_x, k_y, E_{\mathrm{kin}})$ hybrid mode was about 25. It is determined by the number of resolved kinetic energies (here 12) and the transmission factor of the electron optics due to the higher pass energy (500 eV) of the HSA in hybrid mode. The $\alpha^2$- term and the transit time spread due to different path lengths in the HSA are numerically corrected. The performance was validated by studying the well-known electronic structure of Au(111) and Cu(111), including circular dichroism (CDAD) measurements. The high efficiency was exploited in a series of measurements on the Kagome metal $CsV_3Sb_5$.

## O 87: Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy I

Time: Thursday 15:00–17:30 Location: H4

O 87.1 Thu 15:00 H4

**Nonlinear plasmonic near– and far fields in the context of Babinet's Principle** — •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 [1]. 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 nanorod.

However, third harmonic generation (THG) also leads to high temperatures in the structure and its surroundings. These temperatures are usually high enough to destroy more complex samples. Therefore, structures with the same emission properties but a higher ratio of THG to temperature are needed.

To overcome this, we are inspired by the Babinet principle. In this sense, a rod antenna can be replaced by a slit in a thin layer of gold. The surrounding gold should now dissipate heat more effectively than a single rod. This talk compares the (non-linear) emission properties of plasmonic nanostructures and their complementary counterparts, highlighting the applicability of Babinet's Principle.

[1] Wolf, D. *et al.* Shaping the nonlinear near field. *Nat. Commun.* 7:10361 (2016). doi: 10.1038/ncomms10361

O 87.2 Thu 15:15 H4

**Beyond-dipole, self-consistent light-matter coupling in plasmonic cavities from first principles** — •Franco Bonafe[1], Carlos Bustamante[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]MPI for Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, New York, USA

The theoretical treatment of light-matter coupling of molecules in complex electromagnetic (EM) environments is key for making progress in the area of modified matter properties in cavities and strong coupling. While several semiclassical methods can treat the coupling of molecules with EM environments, no method has yet considered the combined effects of self-consistent radiative coupling of molecule and environement, and beyond-electric-dipole interactions to account for the effects of inhomogeneous EM fields. This multiscale problem is now possible to address using our full minimal coupling Maxwell-TDDFT framework [1], implemented in the Octopus package. In this talk, we show how the effects of self-consistent light-matter coupling for different systems. On the one hand, we report the spectral Lamb-like shifts of plasmonic dimers described from first principles when radiation-reaction is considered. Moreover, we discuss the effects of transverse and longitudinal field inhomogeneity in the spectral properties of molecules in plasmonic environments described by a Drude response, including retardation effects. Finally, outlooks on self-consistent coupling of electrons, phonons and structured light are discussed. [1] F.P. Bonafé, A. Rubio, H. Appel et al. arXiv:2409.08959v2 (2024)

O 87.3 Thu 15:30 H4

**Polarisation-dependent Mie void resonances** — •Serkan Arslan[1], Shaban B. Sulejman[2], Sebastian Klein[1], Jonathan Haehner[2], Dominik Ludescher[1], Tim Davis[1,2], Lukas Wesemann[2], Ann Roberts[2], Harald Giessen[1], and Mario Hentschel[1] — [1]Univesity of Stuttgart, 4th Physics Institute, Germany — [2]University of Melbourne, School of Physics & TMOS, Australia

Over the last decade, researchers in nanophotonics have extensively studied the properties and applications of high refractive index dielectric nanoresonators that support subwavelength Mie resonances. Recently, it was demonstrated that similar resonances also occur in wavelength- and subwavelength-sized holes in high refractive index dielectrics, now known as Mie voids. These Mie voids efficiently confine light within air and support resonances spanning from the IR to UV wavelengths, thereby providing a new building block and expanding the parameter space of dielectric nanophotonics.

Until now, only circular Mie voids have been investigated. Here, we present the first study of non-isotropic Mie voids, including elliptical and rectangular shapes. We numerically and experimentally investigate the polarisation dependence of the resonances and reflection spectra, paving the way for polarisation-dependent structural colors and optical security features. Specifically, we demonstrate polarisation-dependent color patterns and micrometer-sized color prints. Anisotropic Mie voids also allow for the design of Mie void metasurfaces based on a generalised geometric phase.

O 87.4 Thu 15:45 H4

**Using strong coupling to control plasmonic catalysis** — •Jakub Fojt, Paul Erhart, and Christian Schäfer — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Plasmonic excitations decay within femtoseconds, leaving nonthermal (often referred to as "hot") charge carriers behind that can be injected into molecular structures to trigger chemical reactions that are otherwise out of reach – a process known as plasmonic catalysis. In this contribution, we demonstrate that strong coupling between resonator structures and plasmonic nanoparticles can be used to control the spectral overlap between the plasmonic excitation energy and the charge injection energy into nearby molecules. Our atomistic description couples real-time density-functional theory self-consistently to an electromagnetic resonator structure via the radiation-reaction potential. Control over the resonator provides then an additional knob for nonintrusively enhancing plasmonic catalysis, here more than 6-fold, and dynamically reacting to deterioration of the catalyst – a new facet of modern catalysis.

O 87.5 Thu 16:00 H4

**Photoemission electron microscopy of Exciton-Polaritons in thin $WSe_2$ waveguides** — •Tobias Eul[1], Victor DeManuel-Gonzalez[1], Miwan Sabir[1], Florian Diekmann[1], Kai Rossnagel[1,2,3], and Michael Bauer[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Ruprecht Haensel Lab, 22607 Hamburg, Germany

Exciton-polaritons emerging from the interaction of photons and excitons in the strong coupling regime are intriguing quasi-particles for the potential exchange of energy during light-matter interaction processes such as light harvesting. This coupling causes an energy anti-crossing in the photon dispersion centered around the exciton resonance, i.e. a Rabi-splitting between a lower and upper energetic branch. The size of this splitting correlates to the coupling strength between the exciton and the photonic modes. In this work, we investigate this coupling between excitons and photonic waveguide modes excited simultaneously in thin-film flakes of the transition-metal dichalcogenide $WSe_2$. Using a Photoemission electron microscope, we are able to extract the dispersion of the TE- and TM-modes propagating through these flakes as well as extract the energy splitting. Ultimately, our findings precipitate the investigation of the propagation of exciton-polaritons in the time-domain via time-resolved photoemission.

O 87.6 Thu 16:15 H4

**Surface-mediated ultra-strong cavity coupling of two-dimensional itinerant electrons** — Christian Eckhardt[1,2], Andrey Grankin[3], Dante Kennes[2,1], Michael Ruggenthaler[1], Angel Rubio[1], •Michael Sentef[4,1], Mohammad Hafezi[3], and Marios Michael[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen University — [3]Joint Quantum Institute, Department of Physics, University of Maryland — [4]Institute for Theoretical Physics, University of Bremen

Engineering phases of matter in cavities requires effective light-matter coupling strengths that are on the same order of magnitude as the bare system energetics, coined the ultra-strong coupling regime. For models of itinerant electron systems, which do not have discrete energy levels, a clear definition of this regime is outstanding to date. Here we argue that a change of the electronic mass exceeding 10% of its bare value may serve as such a definition. We propose a quantitative computational scheme for obtaining the electronic mass in relation to its bare vacuum value and show that coupling to surface polariton modes can induce such mass changes. Our results have important implications for cavity design principles that enable the engineering of electronic properties with quantum light.

O 87.7 Thu 16:30 H4

**Photoheating nanoscale Pd to temperatures exceeding attached Au nanoparticle antennas** — Felix Stete[1], Shivani Kesarwani[2], Charlotte Ruhmlieb[2], Florian Schulz[2], Marc Herzog[1], Holger Lange[1,2], and •Matias Bargheer[1,3] — [1]Universität Potsdam — [2]Universität Hamburg — [3]Helmholtz-Zentrum Berlin

In the non-equilibrium following optical excitation, energy transfer processes at the nanoscale can exhibit extraordinary and surprising phenomena such as heat transport without heating and dominant phonon heat transport in the nobel metal gold. Here we present transient absorption experiments on a systematic and well-characterized series of gold nanoparticles with a Pd satellite shell. Modeling the fluence dependence of the entire series of hybrid structures with a fixed set of thermophysical parameters shows that we can create hybrid nano-photo-catalysts that concentrate light energy into the catalytically active Pd. We can make a few Pd satellites efficiently collect nearly all photothermal energy deposited by plasmonically enhanced absorption in gold and heat up the Pd by 180 K while the gold core remains cold. Consequently, highly active catalytic sites emerge which can enhance light driven molecular transformations. The tailoring and modeling of such unexpected nanoscale energy transfer phenomena is backed up by ultrafast x-ray diffraction experiments that provide a material-specific direct measure of the crystal lattice response to energy in phonons and electrons of each material in heterostructures and nanocomposites.

O 87.8 Thu 16:45 H4

**Investigation of light-matter coupling in tight binding models** — •Jonas Reimann[1,2], Michael Ruggenthaler[1,2], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Center for Computational Quantum Physics, The Flatiron Institute, New York, NY, USA

The theoretical and mathematical foundations for light-matter interactions in a continuum theory are well-established. With the Pauli-Fierz Hamiltonian as the basic building block there is a starting Hamiltonian with all the required properties to study systems containing both matter and light. This can for example be used in the arising field of cavity material engineering where the interplay of light and matter is utilized to design new material properties.

How to imprint these mathematical properties onto tight-binding models describing such materials is at the center of a long-ongoing discussion. A widely deployed approach in this context is the Peierls substitution, coupling light to the hopping elements of the matter Hamiltonian. In this contribution we investigate the reliability of the Peierls substitution in terms of fundamental light-mattter coupling properties within the context of cavity material engineering.

O 87.9 Thu 17:00 H4

**Revealing the crystallization dynamics of phase-change materials in vicinity of metallic nanostructures with multiphysics simulations** — •Luis Schüler[1,2], Lukas Conrads[2], Sebastian Meyer[2], Yingfan Chen[2], Lina Jäckering[2], Matthias Wuttig[2], Thomas Taubner[2], and Dmitry Chigrin[1,2] — [1]DWI - Leibniz Institute for Interactive Materials, Aachen — [2]I. Institute of Physics (IA), RWTH Aachen University, Aachen

Optical metasurfaces composed of metallic or dielectric scatterers (meta-atoms) promise a powerful way of tailoring light-matter interactions. Phase-change materials (PCMs) are prime candidates for non-volatile resonance tuning of metasurfaces based on a change in refractive index. Precise resonance control can be achieved by locally applying laser pulses to crystallize a PCM, modifying the dielectric surrounding of meta-atoms. However, the complex crystallization kinetics of PCMs in the vicinity of metallic meta-atoms have not been studied yet. Here, we investigate metallic dimer antennas on top of the PCM $Ge_3Sb_2Te_6$ and address these nanoantennas with laser pulses to crystallize the PCM below. Our study reveals inhomogeneous crystallization caused by the absorption and heat conduction of the metallic nanoantennas. A self-consistent multiphysics model, including electromagnetic, thermal, and phase-transition processes, is employed to simulate the crystallization and predict the resulting resonance shift of the antennas. This model enables the optimization of the laser parameters and the geometry of the meta-atoms to achieve an optimal resonance shift, thereby improving the efficiency of metasurfaces.

O 87.10 Thu 17:15 H4

**How accurate is the pole expansion of the scattering matrix?** — •Elias Fösleitner[1], Adrià Canós Valero[1], Egor Muljarov[2], and Thomas Weiss[1] — [1]Department of Theoretical Physics, University of Graz, Graz, Austria — [2]School of Physics and Astronomy, Cardiff University, Cardiff, United Kingdom

Optical metasurfaces are flat arrangements of nanostructures with different subwavelength sizes and orientations, which allow tailoring the light propagation in a layer of subwavelength thickness. Such metasurfaces are often described using their resonant states. These states, also known as quasi-normal modes, serve as the foundation for the pole expansion of the optical scattering matrix, providing a more efficient and insightful alternative to conventional full-wave simulations. Existing formulations of such an expansion have, however, limitations, particularly in terms of accuracy, efficiency, and convergence. The aim of this study is to compare different approaches for pole expansions and identify their advantages and limitations. Moreover, we discuss how the choice of basis functions of the scattering matrix influences its complex pole structure and the resulting pole expansion. Overall, these findings will allow for a faster prediction of optical properties by choosing the best suited resonant expansion and also provide additional insight that is necessary for many applications such as nanophotonic sensors.

# O 88: 2D Materials: Stacking and Heterostructures (joint session O/HL)

Time: Thursday 15:00–17:45 Location: H6

O 88.1 Thu 15:00 H6

**Systematic Study of Interlayer Interactions in Transition Metal Dichalcogenide Bilayers Using microARPES** — •Thomas Nielsen[1], Chakradhar Sahoo[1], Alfred Jones[1], Zhihao Jiang[1], Kenji Watanabe[2], Takashi Taniguchi[2], Suman Chakraborty[4], Prasana Sahoo[4], Jill A. Miwa[1], Yong P. Chen[1,3], and Søren Ulstrup[1] — [1]Aarhus University, Denmark — [2]National Institute for Materials Science, Japan — [3]Department of Physics, Purdue University, USA — [4]Materials Science Centre, Indian Institute of Technology, India

Stacked transition metal dichalcogenide monolayers are emerging as a platform to study correlated phases such as Mott insulators or Wigner crystallization. Spatially resolved ARPES can potentially visualize the moiré bands and hybridization effects in the electronic structure underpinning these correlated phases. Observing these phenomena in ARPES in a reproducible way remains challenging, motivating systematic studies of interlayer interactions in twisted TMD bilayers. 20 different heterobilayers of $WSe_2$, $WS_2$, $MoSe_2$, and $WS_2$, as well as homobilayers of $WSe_2$ are fabricated with varying twist angles. Their electronic properties are measured using the microARPES branch at the ASTRID2 synchrotron at Aarhus University. Band alignments and hybridization effects are tracked as a function of material composition and twist angle. The used dry-transfer fabrication techniques do not yield the direct observation of flat bands from moiré effects in the valence band. Based on this work future avenues for reproducibly attaining moiré effects in photoemission from TMDs are discussed.

O 88.2 Thu 15:15 H6

**Gate-Tunable miniband dispersion in twisted graphene superlattices near the magic angle measured with MicroARPES** — •Alfred J. H. Jones[1], Zhihao Jiang[1], Dongkyu Lee[2], Youngji Park[2], Kimberly Hsieh[1], Paulina Majchrzak[1], Chakradhar Sahoo[1], Thomas S. Nielsen[1], Kenji Watanabe[3], Takashi Taniguchi[3], Philip Hofmann[1], Jill A. Miwa[1], Yong P. Chen[1,4], Jeil Jung[2], and Søren Ulstrup[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]Department of Physics, University of Seoul, Korea — [3]National Institute for Materials Science, Japan — [4]Department of Physics and Astronomy, Purdue University, USA

Twisted superlattices of mono- and bilayer-graphene are emerging as powerful tools to explore quantum many-body effects such as unconventional superconductivity and Mott insulating states. Access to the momentum-resolved electronic structure simultaneous to changing the carrier concentration and displacement field within a twisted superlattice device can directly provide key information on the miniband dispersion tunability that underpins the correlated phenomena.

Here, we present microARPES measurements from SGM4 at ASTRID2 on two-terminal "near-magic-angle" twisted bilayer (TBG) and double-bilayer graphene (TDBG) devices. Our findings for the two systems are strikingly different: On TBG, we find a filling factor-dependent bandwidth change of the flat moiré bands, whereas on TDBG the effect of tuning the doping and displacement field leads to non-monotonous bandwidth changes and tunable gap opening effects.

O 88.3 Thu 15:30 H6

**Topological magnetic Moiré heterostructures** — •Aymeric Saunot[1,3], Sebastien E. Hadjadj[2], Tonica Valla[1], Maxim Ilyn[3], and Ilya I. Klimovskikh[1] — [1]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastían, Basque Country, Spain. — [2]Materials Physics Center (MPC), Paseo Manuel de Lardizabal N5,b20018 Donostia, Spain. — [3]Departamento de Física de Materiales UPV/EHU, San Sebastían, Spain.

Over the last few years Moiré superlattices have become a hot topic in condensed matter, thanks to the experimental success of magic angle twisted graphene. Moiré superpotentials arise from either twist or atomic mismatch at the interface between van der Waals materials, leading to a rich physics of strongly correlated electrons. Intriguingly, creation of Moiré pattern on the surface of 3D topological insulator (TIs) is theoretically expected to lead to, among others, topological superconductivity, high Chern number systems and non-trivial magnetic textures. Here, we present Moiré heterostructures made from 3D TIs and novel 2D magnetic insulators transition metal dihalides. We investigate the heterostructure's surface by means of STM, ARPES, XMCD, and LEED. Our results show that the Moiré periodicity and the symmetry of the potential, can be tuned based on the ratio between the lattice parameters of the heterostructure's layers. Band structure measurements excitedly show the main Dirac cone surrounded by several Dirac cone replicas creating new Dirac minicones at the crossing points, opening a whole new platform to study topological Moiré physics.

O 88.4 Thu 15:45 H6

**SNOM of lateral TMDC heterojunctions** — •Philipp Schwendke[1], Samuel Palato[1], and Julia Stähler[1,2] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der MPG

Two transition metal dichalcogenide monolayers, joined together laterally, form a one-dimensional heterojunction where charge transfer with associated space charge region and current rectification have been shown experimentally [1]. Furthermore, there are unique local electronic properties determining the excitonic response in the boundary region. Nanoscale spectroscopic methods are needed for the observation of such local optical properties. We use scanning near-field optical microscopy (SNOM) in combination with a continuous wave (cw) light source at 633 nm, as well as a pulsed laser tunable in a wide range from 250 nm to 1300 nm. We employ pseudo-heterodyne modulation for noise suppression and optical phase information, and quadrature-assisted discrete demodulation in order to use the tunable light source at kHz repetition rates. Resonant SNOM measurements show a quenching near the $WS_2$-$MoS_2$ boundary, which can be indicative of local energy shifts or electronic states specific to the boundary region. This is complementary to previous measurements which show quenching of photoluminescence [2], attributing it to exciton recombination. In addition, the agreement of results acquired with cw and pulsed light sources paves the way towards time-resolved near-field measurements.

[1] Li et al., Science, vol 349, p 524 (2015)

[2] Chou et al., Nanoscale, vol 14, p 6323 (2022)

O 88.5 Thu 16:00 H6

**Charge density wave interactions in bilayer 1T-TaSe2** — •Robert Drost, Ziying Wang, Büşra Arslan, Adolfo Fumega, Jose Lado, and Peter Liljeroth — Aalto University, Department of Applied Physics

Van der Waals materials offer splendid opportunities for quantum material engineering through stacking and heterostructure formation. While well-proven for many essential two-dimensional materials, these techniques are less explored for correlated materials. The 1T phase of TaSe2 is a two-dimensional Mott insulator and and excellent model system for correlations in reduced dimensions. The correlation gap in 1T-TaSe2 is highly sensitive to the thickness of the material, suggesting that electron-electron interactions between the charge density waves play an important role in determining the electronic properties of few-layer TaSe2. We also observe and additional site dependence of the gap size, showing that the stacking order may be equally important. These effects hint at the possibility of using charge density wave stacking as a design element in new quantum materials.

O 88.6 Thu 16:15 H6

**Giant Zeeman effect at a magnetic topological van der Waals interface** — Tobias Wichmann[1,2], Keda Jin[1,3], Jose Martinez-Castro[1,3], Tom G. Saunderson[4,5], Honey Boban[6], Lukasz Plucinski[6], Yuriy Mokrousov[4,5], Markus Ternes[1,3], F. Stefan Tautz[1,2], and •Felix Lüpke[1,7] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]Institut für Experimentalphysik IV A, RWTH Aachen University — [3]Institut für Experimentalphysik II B, RWTH Aachen University — [4]Institute of Physics, Johannes Gutenberg University Mainz — [5]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS), Forschungszentrum Jülich — [6]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich — [7]II. Physikalisches Institut, Universität zu Köln

We report giant Zeeman effects with Landé $g$-factors up to $g \approx 230$ at the interface of graphene and the van der Waals (vdW) ferromagnet $Fe_3GeTe_2$ (FGT). They arise from orbital moments generated by the non-trivial band topology of the FGT and cause a huge asymmetric level splitting when a magnetic field is applied. By exploiting the inelastic phonon gap of graphene, we can directly access the vdW interface to the FGT underneath by scanning tunnelling microscopy and spectroscopy. By analyzing the Faraday-like screening of the tunnelling tip by the graphene, we are able to quantify the electric field at the vdW interface.

O 88.7 Thu 16:30 H6

**Nanoscale band-gap modulation and dual moiré superlattices in the weakly-coupled h-BN/graphite heterostructure** — Fábio J. R. Costa[1,2], Luiz F. Zagonel[1], Tin S. Cheng[3], Jonathan Bradford[3], Christopher J. Mellor[3], Peter H. Beton[3], Sergei V. Novikov[3], Juliette Plo[4], Bernard Gil[4], Guillaume Cassabois[4,5], Klaus Kuhnke[2], Klaus Kern[2,6], and •Anna Rosławska[2] — [1]Unversity of Campinas, Brazil — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]University of Nottingham, United Kingdom — [4]Laboratoire Charles Coulomb, Montpellier, France — [5]Institut Universitaire de France, Paris, France — [6]EPFL, Lausanne, Switzerland

Van der Waals materials, such as hexagonal boron nitride (h-BN), and their heterostructures are highly promising for novel nanophotonic and electronic devices. In such stacks, moiré patterns arise and modulate the electronic properties of the material at the scale of typical superstructure periods (approx. 10 nm), and as such are challenging to probe. Here, we investigate the moiré superlattices in the weakly coupled h-BN/graphite heterostructure at the atomic scale. Scanning tunneling microscopy (STM) imaging reveals extensive moiré unit cells on the surface, while spectroscopic measurements demonstrate significant modulation in the work function and band gap across the periodic supercell. Additionally, we identify a dual moiré superlattice in twisted bilayers of h-BN on graphite, providing an extra degree of freedom to tune the heterostructure's properties.

O 88.8 Thu 16:45 H6

**Impact of point defects and grain boundaries on sulfur diffusion and memristive properties of $MoS_2$ single sheets** — •Aaron Flötotto[1], Jules Oumard[1], Benjamin Spetzler[2], Martin Ziegler[2], Erich Runge[1], and Christian Dressler[1] — [1]Technische Universität Ilmenau, Germany — [2]Christian-Albrechts-Universität zu Kiel, Germany

The memristive properties of transition metal dichalcogenides, such as $MoS_2$, are currently the subject of intense research and have recently been traced back to the dynamics of sulfur vacancies [1, 2]. In this theoretical work, we employ molecular dynamics to determine the sulfur vacancy diffusion coefficients in the vicinity of various point defect structures and grain boundaries in single sheet $MoS_2$. To address the necessity of large cell sizes and long time scales, we utilize machine learning force fields, applying both Gaussian approximation potential and equivariant graph neural networks. We then compare the accuracy of these force fields and discuss the results in regard to the memristive properties of $MoS_2$. Our findings indicate a reduction in energy barriers for sulfur vacancy diffusion as the size of vacancy clusters increases and highlight the importance of certain interstitial sites in these vacancy clusters.

[1] Li, D., et al. (2018). ACS Nano, 12(9), 9240-9252. doi.org/10.1021/acsnano.8b03977

[2] Spetzler, B., et al. (2024). Adv. Electron. Mater., 10, 2300635. doi.org/10.1002/aelm.202300635

O 88.9 Thu 17:00 H6

**Machine-Learning the Electronic Structure of Twisted Bilayer Graphene** — •Lenz Fiedler[1], Agnieszka Kuc[1], Florian Arnold[2], and Attila Cangi[1] — [1]Helmholtz-Zentrum Dresden Rossendorf, Dresden, Deutschland — [2]Technische Universität Dresden, Dresden, Deutschland

Twistronics, i.e., the study of twodimensional materials in which individual layers are twisted w.r.t.õne another, has the potential to significantly propel technological progress. Twisted bilayer materials, e.g., graphene, may exhibit a significant change in electronic structure and electrical properties based on twist angle. Their computational treatment with density functional theory (DFT) proves difficult, as small twist angles affect the periodicity of the cell and can only be simulated with large unit cells. In this talk, the recently introduced Materials Learning Algorithms (MALA) - a framework for accelerating DFT calculations based on machine learning - is applied to twisted bilayer graphene. Bilayer graphene serves as a proxy for the larger field of twistronics itself. It is shown how the electronic structure, including electronic density of states and electronic charge density, can be predicted from a small number of twist angles for a range of twisted bilayer graphene structures. Since the MALA framework uses the local density of states to encode the electronic structure on a numerical grid, predictions can be made on much larger length scales than with standard DFT calculations. This work demonstrates how machine learning can be used to computationally model twisted bilayer structures where standard first-principles methods are not viable.

O 88.10 Thu 17:15 H6

**High-throughput *ab initio* screening of 2D heterostructures** — •Anastasiia Nihei[1,2], Tom Barnowsky[1,2], Roman Kempt[1], and Rico Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Duke University, Durham, USA

Heterostructure interfaces produced by stacking two-dimensional (2D) materials facilitate the development of advanced electronic functionalities down to the atomic level. The efficient autonomous creation and computational study of these systems is, however, a challenge due to the general incommensurability of the 2D monolayers. This often results in large unit cells with hundreds to thousands of atoms.

Here, we present an extensive *ab initio* screening of heterostructures made of 2D systems. The approach makes use of the AFLOW-Hetbuilder – a newly developed tool that automates the heterotructure generation based on coincidence lattice theory [1,2]. It is fully integrated into the AFLOW framework [3,4]. We study the binding energy of a large set of heterostructures and also analyse their structural, electronic, and magnetic properties [5]. The presented efficient workflow can enable the systematic data-driven design of 2D heterostructures.

[1] D. S. Koda *et al.*, J. Phys. Chem. C **120**, 10895 (2016).

[2] https://zenodo.org/record/4721346.

[3] M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023).

[4] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).

[5] A. Nihei *et al.*, manuscript in preparation (2024).

O 88.11 Thu 17:30 H6

**Size-Dependent Diffusion of Radioactive Alcohols Through CNMs** — •Neita Khayya, Andre Beyer, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Conventional membranes frequently struggle to achieve both, high permeance and high selectivity. On the other hand, two-dimensional membranes demonstrated remarkable progress. For example, nanometer-thin carbon nanomembranes (CNMs) from self-assembled monolayers of terphenylthiol molecules combine rapid water permeation with a rejection of ethanol in pressure-driven experiments as well as ultrahigh ionic exclusion in ion conductivity measurements. Although there has been great progress in understanding the distinctive characteristics of CNMs, more work is required to fully understand their transport characteristics, which requires complementary approaches. In this work, we employed the radio-active tracer diffusion method to study the size-depended concentration-driven permeation of different alcohols, namely [14C] CnH2n+1OH (n = 1*3) through thickness-varied CNMs from biphenylthiol (BPT), terphenylthiol (TPT) as well as quaterphenylthiol (QPT) molecules. Our findings align with vaporous alcohol pressure-driven permeation measurements regarding the size exclusion through CNMs. Interestingly, our results indicate an increased permeation rate in the liquid phase, which can be rationalized by hydrogen bonds created inside the membrane between the water molecules and diffused alcohols.

# O 89: Metal and Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Thursday 15:00–17:45 Location: H8

O 89.1 Thu 15:00 H8

**From Unit Cells to Diffraction Patterns: `celltools`, a Python Toolkit for Structural Modeling** — •Sebastian Hammer[1] and Bradley J. Siwick[2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Departments of Physics and Chemistry, McGill University, Montreal H3A 0B8, Canada

The coupling of lattice and electronic system crucially determines the properties of modern materials. This interaction is at the heart of many emergent phenomena, such as charge-density wave formation, polaron dynamics, and transient metal-insulator transitions, which have peaked the interest of researchers.

While electronic properties can often be reliably described by quantum chemical methods, capturing structural changes is computationally more demanding. Hence, diffraction experiments are the usual method of choice to investigate structural distortions. However, extracting atomic positions from diffraction data is tedious and not straight forward.

In this contribution, I introduce the python package `celltools`, a versatile tool for constructing and manipulating unit cells as well as simulating their diffraction patterns. Using the case study of excimer formation in the prototypical molecular semiconductor zinc-phthalocyanine investigated with ultra-fast electron diffraction [1], I demonstrate how this tool enables the extraction of momentary atomic position from time-resolved diffraction datasets.

[1] S. Hammer *et al.*, *PNAS* (2024)

O 89.2 Thu 15:15 H8

**Automation of data acquisition and measurement evaluation in LEED $I(V)$** — •Florian Dörr[1], Michael Schmid[1], Lutz Hammer[2], Ulrike Diebold[1], and Michele Riva[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Solid State Physics, FAU Erlangen, Germany

We designed a system capable of acquiring and evaluating quantitative low-energy electron diffraction [LEED $I(V)$] data, the Vienna Package for Erlangen LEED (ViPErLEED). The system contains three parts: One part performs data acquisition and is discussed in this contribution. The other two parts focus on the extraction of LEED-$I(V)$ curves from image series [1] and simulation of $I(V)$ spectra for quantitative structure optimization [2].

The data acquisition package consists of open-source hardware for controlling the LEED electronics and software for calibration and the actual measurements. Compared with previous solutions, the package contains functions that improve data quality, such as low-noise measurement of the beam current $I_0$, automatic calibration of the beam energy, and analysis of the response time of the LEED controller. On the image acquisition side, the software corrects for deficiencies of the camera, such as hot or dead pixels. We will discuss issues that affect the accuracy and duration of LEED-$I(V)$ measurements; this is especially important for sensitive samples that easily degrade.

[1] https://doi.org/10.48550/arXiv.2406.18413
[2] https://doi.org/10.48550/arXiv.2406.18821

O 89.3 Thu 15:30 H8

**X-ray reflectivity of $\mu$m-samples** — •Steffen Tober[1], Wieland Corts[1,2], Steven Leake[3], Toka Matar[1,2], Lisa Randolph[1], Breno Saraiva[4,5], Vedran Vonk[4], Andreas Stierle[4,5], and Hans-Georg Steinrück[1,2] — [1]Forschungszentrum Jülich, Institute for Sustainable Hydrogen Economy (INW), Jülich — [2]RWTH Aachen, Institute of Physical Chemistry, Aachen — [3]ESRF, Grenoble — [4]Deutsches Elektronen-Synchrotron (DESY), Centre for X-Ray and Nanoscience (CXNS), Hamburg — [5]University of Hamburg, Physics Department, Hamburg

X-ray reflectivity (XRR) non-destructively probes electron density profiles of surfaces and interfaces with sub-nm resolution. Large beam footprints in grazing-incidence geometries commonly limit XRR to mm-sized, flat samples because the beam spillover for smaller samples significantly reduces the signal to noise ratio. To probe samples such as individual particles in electrodes or catalysts, a significant reduction of the footprint is needed. As demonstrated for crystal truncation rods [1], the nm-sized X-ray beams of modern synchrotron sources can be used for XRR on $\mu$m-sized samples with reduced footprint. We present first proof-of-principle studies comparing XRR of mm- and $\mu$m-sized thin-film samples measured with 80 and 400 nm X-ray beams at ESRF ID01 and the necessary optimisation of alignement- and scan procedures [2]. Our results show the general feasibility of nm-beam XRR to be adapted for future *in situ/operando* studies.

[1] J. Stubbs et al., Clays Clay. Miner. 69, 688 (2021)
[2] S. J. Leake et al., J. Synchrotron Rad. 26 571 (2019)

O 89.4 Thu 15:45 H8

**How a quartz crystal microbalance reacts to a thermal load** — Martina Fellinger[1], Eduardo Pitthan[2], Christian Cupak[1], Friedrich Aumayr[1], Daniel Primetzhofer[2], and •Michael Schmid[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Department of Physics and Astronomy, Uppsala University, Sweden

The most common technique for measuring deposition rates in vacuum is the quartz crystal microbalance (QCM). QCMs are also employed for the determination of sputter yields; further applications are in chemistry and biology. In all these applications, the response of the resonance frequency $f$ to temperature is important. Apart from the crystal's sensitivity to a homogeneous temperature [the $f(T)$ curve], the influence of the thermal stress on the frequency has to be taken into account. In contrast to standard AT-cut crystals, SC-cut (stress-compensated) crystals are insensitive to radial stress. Therefore, SC-cut crystals are used for high-precision measurements or if the power dissipated on the crystal is high (e.g., for sputter yield measurements). Nevertheless, stress effects must be taken into account if the heat source is not exactly centered. The static $f(T)$ response and the effects of local heating, including stress effects, lead to a superposition of a fast response (within $\lesssim 1\,\mathrm{s}$) and a slow frequency change over several minutes; the latter being related to the thermal resistance between the crystal and the crystal holder. Examples of finite-element simulations for a localized heat source will be shown and compared to experimental data of SC-cut crystals irradiated by MeV ions with up to 70 mW power, causing a temperature increase by up to 100 K.

O 89.5 Thu 16:00 H8

**Bilayer Formation of Tl on Ag(111): Spatial and Electronic Structural Insights** — •Sarah Laufer[1], Sven Schemmelmann[1], Yuichiro Toichi[2], Kazuyuki Sakamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Applied Physics, Osaka University, Japan

Ultrathin thallium films on Ag(111) have become a model system for studying the spatial and electronic properties of atomic-layer systems [1-3]. In this study, we focus on investigating the formation of bilayer Tl on Ag(111), leveraging Auger electron spectroscopy, low energy electron diffraction (LEED), and inverse photoemission (IPE) to investigate both spatial and electronic structure. LEED studies indicate that the Tl layers are rotated with respect to the substrate, with the angle of rotation depending on the Tl coverage and deposition temperature. Furthermore, IPE measurements reveal distinct unoccupied electronic states for both the monolayer and the bilayer. With increasing deposition time, the intensity of the monolayer-related state is reduced, while the intensity of the bilayer-related state increases. These results provide insight into the bilayer growth mechanism of Tl on Ag(111) and offer experimental criteria for differentiating between mono- and bilayer.

[1] T. Kobayashi *et al.*, Nano Lett. **23**, 7675-7682 (2023)
[2] P. Härtl *et al.*, Phys. Rev. B **107**, 205144 (2023)
[3] S. Schemmelmann *et al.*, Phys. Rev. B **109**, 165417 (2024)

O 89.6 Thu 16:15 H8

**Capping of terbium silicide nanostructures on Si(111)** — •Markus Bachler[1], Milan Kubicki[1], Hüseyin Çelik[2], Sören Selve[3], Martin Franz[1], Michael Lehmann[2], and Mario Dähne[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623, Germany — [2]Institut für Optik und Atomare Physik, Technische Universität Berlin, 10623, Germany — [3]Zentraleinrichtung Elektronenmikroskopie (ZELMI), Technische Universität Berlin, 10623, Germany

Rare earth silicide films on Si surfaces are of great interest because of their appealing properties, such as extremely low Schottky barrier heights on $n$-type Si, abrupt interfaces, and the formation of two- and three-dimensional films or one-dimensional nanowires. However, a protective layer is required for further utilisation of these properties, and capping by Si has the further advantage of no lattice mismatch to the substrate and the opportunity to form three-dimensionally stacked nanostructures. For this purpose, rare earth silicides on Si(111) with their very low to no lattice mismatch to Si are very promising for epitaxial capping.

Here we studied capping of thin Tb silicide layers on the Si(111) surface with Si by using scanning tunneling microscopy, cross-sectional high-resolution transmission electron microscopy as well as cross-sectional scanning transmission electron microscopy with energy dispersive X-ray analysis. We observed that overgrowth of the Tb silicide layers with amorphous and crystalline Si leads to intact double layers, demonstrating the stability of the Tb silicide layer upon capping.

O 89.7 Thu 16:30 H8

**Exploring surface properties of hexagonal Si and Ge** — •Martin Keller[1], Abderrezak Belabbes[1,2], Jürgen Furthmüller[1], Friedhelm Bechstedt[1], and Silvana Botti[1,3] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Sultan Qaboos University, Muscat, Oman — [3]Ruhr Universität Bochum, Germany

We present ab initio calculations, using density functional theory in a slab geometry, that explore structural and electronic properties of the surfaces of hexagonal silicon and germanium, which are novel materials for active optoelectronic applications. We study the relaxed 1 × 1 a, m, c and r-plane facets, who's surface energies allow the creation of Wulff constructions of Si and Ge nanocrystals and wires. Our focus lies on understanding surface stability and its implications on material and device design, as well as the effects of the relaxation on the electronic properties. The comparison with experimental findings offers practical insights for substrate selection for thin film growth and the construction of heterostructures.

O 89.8 Thu 16:45 H8

**Strong electron doping of single-layer $\mathbf{MoS_2}$ on an oxidized contact** — •Marco Bianchi[1,2], Charlotte Sanders[3], Davide Curcio[4], Daniel Lizzit[5], Paolo Lacovig[1], Ezequiel Tosi[6], Jill Miwa[2], Silvano Lizzit[1], and Philip Hofmann[2] — [1]Elettra Sincrotrone Trieste S.C.p.A., Trieste, IT — [2]Dep. of Physics and Astronomy, iNANO, Aarhus University, DK. — [3]Artemis Program, UK Central Laser Facility, Harwell, STFC, UK — [4]IOM, Consiglio Nazionale della Ricerca, Trieste, IT — [5]DPIA - University of Udine, IT — [6]Instituto de Ciencia de Materiales de Madrid (ICMM - CSIC), ES

One of the major obstacles for the use of two-dimensional semiconductors in devices continues to be the high contact resistance to metallic conductors and the associated losses. Promising results have recently been obtained by using group V semimetals as contact materials. The obtained low contact resistance was explained partly by the a degenerate doping of the two-dimensional semiconductor. Here we study the band alignment and structure of such a system, a single-layer of $MoS_2$ on Au(111) with an intercalated layer of Bi. We investigate the electronic structure and growth by angle-resolved photoemission spectroscopy, X-ray photoemission spectroscopy, low energy electron diffraction and scanning tunneling microscopy. Our results show no evidence for an occupation of the $MoS_2$ conduction band when the material is brought into close contact with Bi. Surprisingly, however, a subsequent oxidation of the intercalated Bi gives rise to an extremely strong electron doping of the conduction band with a carrier density on the order of $10^{13}$ cm$^{-2}$.

O 89.9 Thu 17:00 H8

**Growth of two-dimensional Ta-S structures from $\mathbf{TaS_3}$ nuclei to TaS islands** — •Catherine Grover[1], Alice Bremerich[1], Kai Mehlich[1], Abdus Samad[2], Udo Schwingenschlögl[2], Carsten Busse[1], and Thais Chagas[1] — [1]Department Physik, Universität Siegen, D-57072 Siegen, Germany — [2]Physical Science and Engineering Division, King Abdullah University of Science and Technology, 23955-6900 Thuwal, Saudi Arabia

Transition metal dichalcogenides (TMDCs) are emerging as promising 2D materials, known for their unique physical and electronic properties. Despite the rapid growth of research in this field, the exact mechanisms governing their growth remain largely speculative, especially when compared to more well-understood systems, such as metal-on-metal growth.

In this study, we employ Scanning Tunneling Microscopy (STM) to investigate the growth process of ultrathin tantalum sulfide (Ta-S) phases. We observe the evolution from embedded $TaS_3$ nuclei to $Ta_3S_6$ islands, and ultimately to TaS islands. These findings provide new insights into the growth dynamics of Ta-S phases, revealing the underlying processes.

Furthermore, these structural observations are supported by Density Functional Theory (DFT) calculations, which compare the energies of various structures, offering additional validation of the experimental results.

O 89.10 Thu 17:15 H8

**Ab initio surface phase diagram of $\mathbf{(Al_xGa_yIn_{1-x-y})_2O_3}$** — •Qaem Hassanzada[1], Yuanyuan Zhou[1,2], and Matthias Scheffler[1] — [1]The Fritz Haber institute, Berlin, Germany — [2]The Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Group III sesquioxides with ultra-wide bandgaps are the most promising candidates for high-power electronics. Numerous efforts have been made to grow group-III sesquioxides, however, the fundamental understanding of growth process is still shallow. The prerequisite to understand growth process is detailed information about the surface geometry and stoichiometry under growth conditions. This can be provided in surface phase diagrams. In this study, we explore the surface phase diagram of Group III sesquioxides, $(Al_xGa_yIn_{1-x-y})_2O_3$, for the entire compositional range, using ab initio atomistic thermodynamics [1, 2] and the sure-independence screening and sparsifying operator (SISSO) [3] machine learning methods. We predict the most probable phases under the corresponding growth conditions. For instance, in the Ga-rich region, we predict the formation of a Ga monolayer, which may be related to the experimental hypothesis of Ga adlayer formation at a lower O/Ga ratio [4] reminiscent of the phenomena in GaN.

[1] Scheffler, M. Studies in Surface Science and Catalysis, Vol. 40; Elsevier: 1988, pp 115−122. [2] Reuter, K.; Scheffler, M. Phys. Rev. B 2001, 65, 035406. [3] Ouyang, R. et al. M. Phys. Rev. Mater. 2018, 2, 083802. [4] Chou, T. et al. AIP Advances 2021, 11, 115323.

O 89.11 Thu 17:30 H8

**Ultrathin NiO(100) films on Ag(100): Pitfalls in understanding growth using intensity-voltage low-energy electron diffraction** — •Jan Lachnitt[1], Shuvankar Das[2], Krishnakumar S. R. Menon[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]Surface Physics & Material Science Division, Saha Institute of Nuclear Physics, Kolkata, India

Ultrathin NiO films have prospective applications in heterogeneous catalysis, microelectronics, and spintronics and are thus an object of active research. In model systems, the Ag(100) surface is frequently used as support for these films, as its cubic lattice parameter is only 2.2% smaller than that of NiO, enabling pseudomorphic growth for very small thicknesses. Interestingly, the early-stage growth of NiO films on Ag(100) turns out to be complex compared to other simple oxide systems, such as MgO/Ag(100). We have grown pseudomorphic NiO(100) films of well-defined average thickness in steps of 0.5 monolayer (ML), up to 3 MLs, and studied them with intensity-voltage low-energy electron diffraction (IV-LEED). We have also employed density-functional theory (DFT) calculations to gain additional insights. Our IV-LEED results indicate a deviation from layer-by-layer growth, expected to take place from 2 MLs onwards [1], and the detailed analysis of the oxide-metal system has turned out to be tricky. We discuss the pitfalls and limitations of common IV-LEED procedures and compare the results with our DFT calculations and existing literature.

[1] J. Wollschläger et al., Thin Solid Films 400 (2001) 1.

# O 90: Spins on Surfaces at the Atomic Scale II

Time: Thursday 15:00–17:30 Location: H11

O 90.1 Thu 15:00 H11

**Relativistic Orbital Effects in Hyperfine Splittings on Surfaces** — •Katharina Lorena Franzke, Wolf Gero Schmidt, and Uwe Gerstmann — University of Paderborn Warburger Str. 1 33098 Paderborn

The recent combination of electron spin resonance and scanning tunneling spectroscopy (ESR-STM) provide a new platform to access single spins of atoms and molecules on surfaces [1, 2]. Characteristic hyperfine (hf) splittings due to the interaction between the electronic spin and the magnetic moments of the nuclei can be measured and compared with theoretical predictions from density functional theory (DFT). In comparison with defects in bulk material, however, the calculated data deviates considerably from the experimental values. Limited accuracy of the xc functionals or the direct influence of the electric field of the STM-tip have been discussed as possible reasons.

Large parts of the observed discrepancies however stem from a relativistic effect, the suppression of orbital quenching at surfaces. We developed a fully relativistic method that allows the calculation of this orbital contribution for complex structures [3]. For Pb ions as well as PbPc molecules on the MgO/Ag(111) substrate, this orbital part leads to additional hf splittings in the GHz range and is thereby required to achieve overall accuracy in predicting the hf interactions of single spins in 2D nanostructures.

[1] S. Baumann, et al., Science 350, 417 (2015) [2] L. Farinacci et al., Nano Letters 22, 8470 (2022) [3] K.L. Franzke, et al. J. Phys.: Conference Series. 2701, 012094 (2024)

O 90.2 Thu 15:15 H11

**Electric Control of Molecular Spins on a Surface** — •Paul Greule[1], Wantong Huang[1], Máté Stark[1], Kwan Ho Au-Yeung[1], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], Christoph Wolf[2], and Philip Willke[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Korea

Single electronic spins hosted by atoms or molecules are candidates for future quantum technologies. To utilize them as functional building blocks in quantum information processing it is necessary to gain local control of their quantum properties. Lately, electron spin resonance combined with scanning tunnelling microscopy (ESR-STM) was demonstrated as a versatile method to access atoms and molecules on a surface [1]. For single Ti atoms it was shown that the Zeeman energy of electron spins can be tuned via the applied bias voltage in the tunnelling junction [2] constituting an atomic-scale electric field control. In our work, we present a voltage-dependent shift of the ESR frequency for two different molecular spin systems, Iron-phthalocyanine (FePc) and FePc-Fe ferrimagnet complexes. Intriguingly, we observe a strong non-linearity in the shift connected to the molecular orbital of FePc. We rationalize this theoretically by many-body interactions with the exchange bias field of the tip. Moreover, we show how the bias voltage control can be used to detune Rabi oscillations in pulsed ESR experiments. [1] Y. Chen et al., Adv. Mater. 2022, 2107534 [2] P. Kot et al., Nat Commun 14, 6612 (2023)

O 90.3 Thu 15:30 H11

**Coherent control of a single Er electron spin on surface** — Dasom Choi[1,2], Yaowu Liu[1,3,4], Stefano Reale[1,3], Jeongmin Oh[1,2], We-hyo Seo[1,3], Andreas Heinrich[1,2], Soo-hyun Phark[1,3], and •Fabio Donati[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Korea — [2]Physics Department, Ewha Womans University, Korea — [3]Ewha Womans University, Seoul, Korea — [4]Department of Energy, Politecnico di Milano, Milano, Italy

Electron spins on surface provide an atomic scale qubit platform for quantum information science using scanning tunneling microscopy (STM) [Phark et al. ACS Nano 17, 14144 (2023), Wang et al. Science 382, 87 (2023)]. A bottleneck of this new platform lies in the decoherence stemming from the strong interaction with the environments. Lanthanide atoms, with their highly localized 4f electrons, offer a potential solution to this issue and make them as strong candidates of single atomic spin qubits on surfaces with a high quality factor $Q = 2\Omega T_2$ ($\Omega$ = Rabi rate, $T_2$ = coherence time). In this talk, we present a recent advance in the qubit quality factor, achieved using erbium (Er) atoms on a MgO surface [Reale et al. Phys. Rev. B 107, 045427 (2023)]. We performed a coherent control of the Er atoms using pulsed electron spin resonance (ESR), sensed by a nearby Ti spin [Reale et al. Nat. Commun. 15, 5289 (2024)]. Notably, a single Er spin showed a fivefold improvement in the qubit quality factor compared to the prototypical Ti spin on the same substrate [Yang et al. Science 366, 509-512 (2019)]. This result represents a step towards implementing quantum processes into atomic spin qubits on surfaces.

O 90.4 Thu 15:45 H11

**Spin interactions at the periphery between atomic and condensed-matter physics** — •Dmitriy Borodin, Andrés Pinar Solé, Merve Ercelik, and Andreas J. Heinrich — IBS Center for Quantum Nanoscience, Seoul, South Korea

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 coexists, ultimately defining the local magnetic structure and phase stability. In this work, we use low-temperature scanning probe microscopy to investigate the exchange mechanisms and interaction energies between atoms on surfaces and magnetic tips. By controlling the atom-tip separations on a picometer scale, we can continuously tune the interaction energies and observe changes in the local magnetic structure of the tip. Furthermore, we explore the impact of the elemental composition of magnetic tips on their exchange interactions with surface-bound atoms and identify experimental strategies to adjust the sign and strength of these interactions.

O 90.5 Thu 16:00 H11

**Switching Dynamics in Fe Spin Chains: Quantum vs. Classical Behavior** — •Henrik Lichtl[1], Lukas Veldman[1], Johannes Schust[1], Nicolaj Betz[1,2], Laëtitia Farinacci[1,3], 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]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena - Stuttgart - Ulm, Germany

That quantum spins transition to classical magnets at a certain size is well-known, but the behavior of magnets at this transition point has remained elusive. Here we develop a method to measure high speed magnetization curves in a scanning tunneling microscope (STM) that reach magnetic field sweep rates up to kT/s. This allows us to measure the magnetization reversal of antiferromagnetic few-atom spin chains, constructed of Fe atoms on a Cu2N surface. By resolving the statistics of the quantum jumps between the antiferromagnetic ground states, we can clearly distinguish between classical and quantum regimes of magnetic switching. Quantum mechanical behavior quenches rapidly with increasing size such that chains of more than five atoms in length can behave as classical magnets. The ability to modulate spin systems at high speed brings techniques that were previously reserved for bulk measurements to the atomic scale and provides deep insights into the coupling mechanisms between quantum spins and their environment.

O 90.6 Thu 16:15 H11

**Many-body effects in impurity spectroscopy using ESR-STM** — •Christoph Wolf[1,2], Xue Zhang[3], Jose Reina-Galvez[1,2], Jan Martinek[4], and Nicolas Lorente[5,6] — [1]Center for Quan tum Nanoscience, Institute for Basic Science (IBS), Seoul, Korea — [2]Ewha Womans University, Seoul, Korea — [3]Spin-X Institute, China University of Technology, Guangzhou, China — [4]Institute of Molecular Physics, Polish Academy of Science, Poland — [5]Centro de Fisica de Materiales, CFM/MPC (CSIC-UPV/EHU), Spain — [6]6Donostia International Physics Center (DIPC), Spain

Recent advances in understanding how harmonic electric fields drive coherent spin transitions in the ESR-STM have lead to a re-evaluation of experimentally observed phenomena in the ESR-STM spectra of atomic and molecular spin adsorbed on ultrathin insulating layers. In this talk, I will show the most up to date development of our transport approach, which is based on a single-orbital Anderson impurity model attached to magnetic leads. I will focus on two aspects: first, the DC bias control of the resonance frequency of the ESR transition, which can be interpreted as an exchange bias field. This allows the full physical characterization of the adsorbate spin and the junction parameters in ESR-STM. All simulations are qualitatively and quantitatively evaluated against experimental data of individual titanium atoms and Iron(II)phthalocyanine molecules which are prototypical spin-1/2 qubits. Second, I will discuss the optimization of quantum-coherent control in the low-current regime, which shows a distinct optimum for the quantum-bit figure of merit $\Omega$T2.

O 90.7 Thu 16:30 H11

**Driving nuclear spin transitions on a single atom using STM** — •Cristina Mier Gonzalez, Hester Vennema, Evert Stolte, Jinwon Lee, and Sander Otte — Delft University of Technology, 2628 CJ Delft, The Netherlands

Nuclear spins are highly isolated from its electronic environment compared to electron spins. This degree of isolation makes nuclear spins a promising platform for quantum technologies [1]. The development of ESR-STM has made possible the indirect measurement of nuclear spins on single atoms through the hyperfine interaction [2]. More recently, single-shot read-out on Ti isotopes has shown a nuclear lifetime of about 5 seconds [3].

In this work we aim to controllably address nuclear spin transitions using ESR-STM. We propose a double resonance measurement scheme to controllably drive the nuclear spin of a $^{47}$Ti isotope ($I = 5/2$). Our study paves the way for coherent manipulation of single nuclear spins using STM.

[1] J. Pla et al. Nature 496, 334-338 (2013).
[2] P. Willke et al. Science 362, 336-339 (2018).
[3] E.W. Stolte et al. arXiv:2410.0870 (2024).

O 90.8 Thu 16:45 H11

**Single-shot readout of an individual nuclear spin using a scanning tunnelling microscope** — •Evert Stolte[1], Jinwon Lee[1], Hester Vennema[1], Rik Broekhoven[1], Esther Teng[1], Allard Katan[1], Lukas Veldman[2], Philip Willke[3], and Sander Otte[1] — [1]Department of Quantum Nanoscience, TU Delft — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart — [3]Physikalisches Institut, Karlsruhe Institute of Technology

Nuclear spins owe their long-lived magnetic states to their excellent isolation from the environment. At the same time, a limited degree of interaction with their surroundings is necessary for reading and writing the spin state. Therefore, detailed knowledge of and control over the atomic environment of a nuclear spin is key to optimizing conditions for quantum information applications. Scanning tunnelling microscopy (STM), combined with electron spin resonance (ESR), provides atomic-scale information of individual nuclear spins via the hyperfine interaction. However, STM has thus far only sparingly been used to investigate nuclear spins in the time domain. As such, no nuclear spin lifetimes have yet been reported. Here, we demonstrate single-shot readout of an individual $^{49}$Ti nuclear spin with an STM. Employing a pulsed measurement scheme, we find its lifetime to be in the order of seconds. Furthermore, we shed light on the pumping and relaxation mechanisms of the nuclear spin by investigating its response to both ESR driving and tunnelling current. These findings give an atomic-scale insight into the nature of nuclear spin relaxation and are relevant for the development of atomically assembled qubit platforms.

O 90.9 Thu 17:00 H11

**Spin Excitations of High-Spin Fe(II) in Metal-Organic Chains on Metal and Superconductor** — •Jung-Ching Liu[1,2], Chao Li[2], Outhmane Chahib[2], Xing Wang[3], Simon Rothenbühler[4], Robert Häner[4], Silvio Decurtins[4], Ulrich Aschauer[5], Shi-Xia Liu[4], Ernst Meyer[2], and Rémy Pawlak[2] — [1]Department of Physics, Technical University of Munich, James-Franck-Str.1, 85748 Garching, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland — [4]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland — [5]Department of Chemistry and Physics of Materials, University of Salzburg, Jakob-Haringer-Strasse 2A, 5020 Salzburg, Austria

Magnetic anisotropy induced by the substrate plays an important role in many-body interactions in metal-organic frameworks at surfaces. Investigated by STM at 1K, we present the study of magnetic signature at Fe atoms with high spin-state (S=2) using PTO as ligands. On Ag(111), we found long-range Fe-Fe coupling in addition to low-energy spin-flip excitations. Despite of the identical chain structure, such long-range superexchange through PTO is not observed on tunneling spectra on Pb(111) superconductor. We ascribe this distinct spin-spin coupling behavior to the depletion of electronic states around the Fermi level on Pb(111) as compare to Ag(111). We believe our study provides a route for fundamental studies in spin-spin and spin-substrate interactions with different lattice structures.

O 90.10 Thu 17:15 H11

**Control of the Landau-Zener Gap in Atomic Structures** — •Piotr Kot[1,2], Yaowu Lei[1,2], Valeria Sheina[1,2], We-hyo Seo[1,2], Andreas Heinrich[1,2], and Soo-hyon Phark[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, South Korea — [2]Department of Physics, Ewha Womans University, Seoul, South Korea

Avoided crossings in quantum systems have been shown to be a useful tool for the study of qubits and the actualization of faster qubit operations. This is done by taking advantage of Landau-Zener transitions, allowing one to measure quantum interferometric effects. However, implementing these techniques in on surface atoms has not yet been demonstrated experimentally, and is a crucial next step for studying this new class of spin qubits. Here we present preliminary steps towards studying quantum interferometric effects in Ti dimers using electron spin resonance scanning tunnelling microscopy. Firstly, we have fine-tuned the Landau-Zener gap in our dimers by studying the dipole and exchange interaction between the atoms. We have found that only several dimers have the correct gap magnitude for our experimental conditions. Secondly, we have found that by using three atom structures we are able to position the avoided crossing within our range of interest. Experiments in the near future will include measuring Landau-Zener transitions, Stueckelberg oscillations and quantum interferometry maps.

# O 91: Focus Session Chemical Imaging for the Elucidation of Molecular Structure I (joint session O/BP)

Unravelling the multiscale molecular heterogeneity at interfaces is one of the main challenges in modern biophysics and surface science due to the major role specific structural properties play in determining their macroscopic function and behavior. In the last few decades, several specialized chemical imaging techniques have been developed that can reveal many of these crucial structural details, representing an enormous advance in our elucidative capabilities. Clear examples of this range from super-resolution and 3D tomography to tag-free characterization down to the single-molecule level. This focus session will explore the vast range of methods and possibilities for characterizing the different structural aspects in heterogeneous molecular systems and specifically highlight the potential complementarity of the different techniques through multi-modal approaches. Overall, by bringing together different communities, this session aims to foster scientific exchanges that could spark the next major developments in chemical imaging.

Organized by
Martin Thämer (FHI Berlin), Alexander Fellows (FHI Berlin), and Kerstin Blank (University Linz)

Time: Thursday 15:00–17:30 Location: H24

**Invited Talk** O 91.1 Thu 15:00 H24

**Infrared Nanoscopy and Tomography of Intracellular Structures** — Joachim Heberle[1], Katerina Kanevche[1], •Emmanuel Pfitzner[1], David Burr[2], Janina Drauschke[2], Andreas Elsaesser[2], and Jacek Kozuch[1] — [1]Freie Universität Berlin, Department of Physics, Experimental Molecular Biophysics, — [2]Experimental Biophysics and Space Sciences, Arnimallee 14, 14195, Berlin, Germany

Although techniques such as fluorescence-based super-resolution imaging or confocal microscopy simultaneously gather morphological and chemical data, these techniques often rely on localized and chemically specific markers. To eliminate this flaw, we have developed a method of examining cellular cross-sections using the imaging power of scattering-type scanning near-field optical microscopy (sSNOM) and Fourier-transform infrared spectroscopy at a spatial resolution far beyond the diffraction limit (nanoFTIR). Herewith, nanoscale surface and volumetric chemical imaging are performed using the intrinsic contrast generated by the characteristic absorption of mid-infrared radiation by the covalent bonds. We employ infrared nanoscopy to study the subcellular structures of eukaryotic (C. reinhardtii) and prokaryotic (E. coli) species, revealing chemically distinct regions within each cell. Serial 100 nm-thick cellular cross-sections were compiled into a tomogram, yielding a three-dimensional infrared image of subcellular structure distribution at 20 nm spatial resolution. The presented methodology can image biological samples with less interference due to the low energy of infrared radiation and the absence of labeling.

**Invited Talk** O 91.2 Thu 15:30 H24

**Coherent Raman Imaging** — •Michael Schmitt[1] and Juergen Popp[1,2] — [1]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, Helmholtzweg 4, 07743 Jena, Germany — [2]Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Albert-Einstein-Straße 9, 07745 Jena, Germany

Raman-based technologies have profoundly impacted life sciences and biomedical research. Despite their unmatched molecular specificity, traditional Raman spectroscopy suffers from limited sensitivity, making it less suitable for rapid imaging. This limitation is addressed by coherent Raman scattering (CRS) microscopy, primarily through coherent anti-Stokes Raman scattering (CARS) and stimulated Raman scattering (SRS). This talk examines the potential of CARS and SRS imaging for biological and biomedical analysis, offering detailed insights into the molecular composition of biomedical specimens, such as cells or tissue. The presentation will focus on the applications of these techniques in molecular and functional diagnostics in the fields of medicine and life sciences. Furthermore, recent developments in translating CRS into compact, clinically viable systems, such as handheld probes, will be presented, focusing on intraoperative tumour diagnostics for early detection and improved improved therapeutic outcomes.

**Acknowledgement:** Financial support of the EU, the *Thüringer Ministerium für Wirtschaft, Wissenschaft und Digitale Gesellschaft*, the *Thüringer Aufbaubank*, the BMBF, the DFG, and the Carl Zeiss Stiftung is acknowledged.

**Invited Talk** O 91.3 Thu 16:00 H24

**Sum Frequency Generation Microscopy of Electrochemical Interfaces** — •Steven Baldelli — University of Houston, Houston, Texas

Sum frequency generation spectroscopy (SFG) is a valuable technique to study the molecular properties of surfaces. As a second-order technique, it is uniquely sensitive to the average organization of molecules at the surface. However, as most surfaces are spatially heterogeneous, it isn't easy to interpret the spectrum as a single domain. The development of SFG into microscopy has allowed a more detailed and accurate analysis of the spatio-spectro-temporal evolution of surface chemistry. The SFG microscope development will be presented, and compressive sensing and the application toward electrocatalysis will be used.

O 91.4 Thu 16:30 H24

**Elucidating the Composition, Order, and 3D Molecular Orientation of Thin Films with Phase-Resolved Sum-Frequency Generation Microscopy** — •Alexander Fellows, Ben John, Martin Wolf, and Martin Thämer — Fritz-Haber-Institute, Berlin, Germany

The vast majority of molecular interfaces have highly heterogeneous structures, ranging across all length-scales. These manifest as variations in density, composition, and molecular packing structure, all of which are critical in controlling the macroscopic properties and functional behaviour of the films. While various chemical imaging techniques can access many of these important structural details, characterising their relative order and specific packing arrangements represents a formidable challenge.

Here, we present a chemical imaging approach based on phase-resolved sum-frequency generation (SFG) microscopy. By probing molecular vibrations, this technique achieves molecular recognition and thus is sensitive to the local composition and density. Furthermore, through its symmetry selection rules, output SFG signals are dependent on absolute molecular orientations. This hence allows it to distinguish different molecular conformations and characterise the amount of orientational order in the system. Finally, with an azimuthal-scanning approach, the in-plane and out-of-plane signal contributions can be separated, allowing the 3D molecular orientations to be elucidated. By applying SFG imaging to model lipid monolayers, we gain an unprecedented overview of their hierarchical packing structures.

O 91.5 Thu 16:45 H24

**Low temperature multimode atomic force microscopy using an active MEMS cantilever** — Michael G. Ruppert[1], Miguel Wiche[2], André Schirmeisen[2], and •Daniel Ebeling[2] — [1]University of Technology Sydney, Australia — [2]Justus Liebig University Giessen, Germany

Low-temperature atomic force microscopy (AFM) is one of the most powerful tools in surface science. With the chemical bond imaging technique, i.e., by using CO functionalized AFM tips, it became possible to visualize the chemical structure of individual organic molecules, which is essential for studying on-surface reactions and molecular manipulation processes. Routinely, such measurements are performed with qPlus sensors. Here, we present a proof of concept for an active microelectromechanical systems (MEMS) microcantilever with integrated piezoelectric sensing and demonstrate its capability to obtain scanning tunneling microscopy as well as high-resolution non-contact atomic force microscopy images on an atomically flat Au(111) surface. Equipped with a focused ion beam deposited tungsten tip, the active MEMS cantilever is able to obtain high contrast scanning tunneling and frequency shift images at the fundamental and a higher eigenmode of the cantilever. This is interesting for the application of multifrequency AFM operation modes that could enhance the capabilities of the bond imaging technique.

O 91.6 Thu 17:00 H24

**Instrumentation for high-resolution biomolecule imaging enabled by electrospray ion beam deposition (ES-IBD)** — •Lukas Eriksson[1], Tim Esser[1,2], and Stephan Rauschenbach[1] — [1]University of Oxford, Oxford, UK — [2]Thermo Fisher Scientific, Eindhoven, Netherlands

Direct imaging of (bio-)molecules with cryogenic electron microscopy (cryo-EM) or scanning probe microscopy (SPM) is a powerful approach for elucidating molecular structure. However, sample preparation can be a major challenge: either very time- and resource-intensive or incompatible with the vacuum environment required by the imaging method.

Here, we explore preparative mass spectrometry as an alternative workflow towards structural elucidation of biomolecules. A novel, custom-built deposition stage extending a commercial mass spectrometer (Thermo Fisher Scientific Orbitrap UHMR) allows for the mass-filtered, soft-landed deposition of a wide mass range of target molecules ($m = 100$ to $10^6$ Da) onto various surfaces, including cryo-EM grids and metal crystals for SPM. Successful deposition and subsequent imaging requires extensive control over conditions such as pressure, temperature, ion trajectories, sample surfaces, and sample transfer to obtain clean, chemically pure samples of the desired species in the right (i.e. native) configuration. The sample holder also enables controlled growth of ice layers for embedding deposited molecules, allowing high-resolution reconstructions of proteins from cryo-EM.

O 91.7 Thu 17:15 H24

**LFM study of copper oxide** — •Sophia Schweiss, Alfred J. Weymouth, and Franz J. Giessibl — Universität Regensburg, Regensburg, Deutschland

Small-amplitude FM-AFM is a method to study surfaces and adsorbates with atomic resolution. At low temperature, the tip apex can be prepared so that it ends in a single O-atom, making the tip inert and enhancing imaging [1, 2]. With a laterally oscillating tip, i.e. lateral force microscopy (LFM), the conservative (frequency shift, $\Delta f$) and non-conservative (dissipated energy, $E_{\text{diss}}$) components of the tip-sample interaction can also be independently measured. Here too, inert tip apices are commonly used. One measurement of $E_{\text{diss}}$ relies on the cocking and snapping of the tip over a single chemical bond, for which the current state of the art utilizes CO-terminated tips. In this work, a CO-terminated tip [1] is used to investigate the $(2 \times 1)$O reconstruction of Cu(110) with LFM. Simulations are performed to guide interpretation. In this larger ongoing study, these LFM measurements will be repeated for a CuOx tip [2] to evaluate it as a tool for measuring $E_{\text{diss}}$.

[1] Gross et al., Science, **325**, 1110 (2009)
[2] Mönig et al., Nat. Nano., **13**, 371 (2018)

## O 92: Electronic Structure Theory

Time: Thursday 15:00–18:15 Location: H25

O 92.1 Thu 15:00 H25

**Electronic and Optical properties of K-Sb and Na-Sb binary crystals from ab initio many-body theory** — •Richard Schier and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institut für Physik

Alkali-based photocathode materials have come into the limelight as novel semiconducting materials for electron sources. However, challenges in sample purity and polycrystallinity hinder the direct experimental determination of their intrinsic properties. First-principles methods can effectively complement experiments in predicting favorable structures and gaining insight into their electronic and optical properties. In this work, we investigate K-Sb and Na-Sb binary crystals emerged as stable phases from high-throughput screening [1]. Using many-body perturbation theory on top of density functional theory, we find that all considered materials have optical gaps in the near-infrared region between 0.7 - 1.2 eV. The character of the excitations and electron-hole correlations therein are highly dependent on the composition and crystal structure of the compound. Excitonic effects appear more pronounced in the K-Sb crystals, where binding energies are of the order of 100 - 200 meV and the oscillator strength is sizably redistributed to lower-energy peaks. These characteristics indicate that K-Sb crystals are favorable candidates for efficient electron sources. [1] R. Schier, D. Guo, H.-D. Saßnick, and C. Cocchi, Adv. Theory Simulations (2024), https://doi.org/10.1002/adts.202400680.

O 92.2 Thu 15:15 H25

**Automated Wannier functions inspired by topological quantum chemistry** — •Stepan S. Tsirkin — Centro de Física de Materiales, San Sebastián, Spain

Despite Wannier functions (WFs) becoming a popular and powerful technique for studying diverse electronic properties of materials, the construction of high-quality WFs remains a non-trivial task, often requiring manual intervention and expertise, which obstructs high-throughput calculations using WF-based methods.

I present an approach for selecting initial projections for Wannier functions based on the symmetry indicators of DFT bandsstructure. The initial projections are searched among the possible orbitals at the Wyckoff positions of the crystal, referred to as Elementary Band Representations in the terminology of Topological Quantum Chemistry [Nature 547, 298 (2017)]. Thus, the projections are by construction compatible with the symmetry of the bands, making them suitable for the construction of symmetry-adapted WFs (SAWFs) [Sakuma, PRB 87, 235109 (2013)]. This approach has been implemented in the codes WannierBerri (WB) [NPJ Comput. Mater. 7, 33 (2021)] and IrRep [CPC 272, 108226 (2022)]. Additionally, WannierBerri now implements the construction of SAWFs without several limitations found in the corresponding implementation in Wannier90. In particular, WB can handle spin-orbit coupling, a frozen window, and is compatible with multiple DFT codes (VASP, Quantum Espresso, Abinit, etc.).

This method does not require manual inspection on bands, which makes it suitable for high-throughput calculations.

O 92.3 Thu 15:30 H25

**Learning conductance of aromatic and antiaromatic molecular junctions** — •Mohammad Ali Mohammadi Keshtan and Hector Vazquez — Inst. of Physics, Czech Academy of Sciences

Single-molecule junction conductance depends on molecular conformation. The standard computational method to study the conductance of a molecular junction is DFT-NEGF. However, DFT-NEGF is computationally expensive, so finding a fast and accurate method to compute the conductance of a large numbers of structures is vital.

Here, we use machine learning (ML) methods, including kernel ridge regression and Gaussian process regression, to overcome these limitations. To train the regression models, we first generate thousands of junction geometries using classical molecular dynamics at room temperature. For each geometry we then compute conductance using a computationally efficient approximation which considers a Au-molecule-Au complex [1], and build SOAP and Coulomb matrix descriptors.

We study a pair of aromatic/antiaromatic porphyrin-like molecules [2], whose large size further hampers the use of DFT-NEGF. We explore the performance of the different ML models, compare the results with DFT-NEGF, and discuss the relative importance of the different descriptors. Our work demonstrates how ML models can be efficiently trained and used to compute single molecule junction conductance.

[1] H. Vazquez, J. Phys. Chem. Lett. 2022, 13, 9326
[2] S. Fujii et al., Nat. Commun. 2017, 8, 15984

O 92.4 Thu 15:45 H25

**Electronic excitations in nanostructures from the Bethe-Salpeter equation** — •Maximilian Graml, Štěpán Marek, and Jan Wilhelm — Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany

Electronic structure calculations are a well-established tool for the identification of candidate materials for technological applications, e.g., in photocatalysis, photovoltaics and energy storage. For the quantitative description of optical properties, many-body perturbation theory within the GW approximation and the Bethe-Salpeter equation (BSE) on top of GW is regarded as the state-of-the-art method.

In this contribution, we present the implementation of the BSE within the open-source package CP2K, enabling the accurate calculation of electronic excitations in molecules and nanostructures. To validate our approach, we benchmark the excitation energies against those obtained with the FHI-aims package.

We further apply our BSE implementation to study electronic excitations in graphene nanostructures, where we investigate the optical absorption spectra and the spatial extent of excited states as a function of nanostructure size. We observe that both properties converge on the scale of 5 nm nanostructure size, guiding experiments towards the rational design of nanostructures in graphene-based optical devices.

O 92.5 Thu 16:00 H25

**Electronic Coupling on Surfaces from First-Principles: Chemisorped Systems** — •Simiam Ghan and Jens Nørskov — Technical University of Denmark DTU

We use density-functional theory to calculate the electronic coupling matrix elements between adsorbates and surfaces, applying a recently developed diabatization method[1] to fully chemisorped systems. The scheme is demonstrated by calculating ultrafast electron transfer lifetimes within a Fermi golden rule framework, which compares favorably to core-hole-clock measurements for systems including Black Phosphorous, S/Ru(0001) and CO/Ru(0001). We thereby demonstrate the suitability of diabatization schemes for the description of coupling in chemisorped systems, enabling an advantageous interpretation of the electron transfer process. We discuss prospects for the use of first-principles coupling matrix elements to describe other surface phenomena, such as chemisorption and heterogenous catalysis, e.g. within Newns-Anderson models.

[1] S. Ghan *et al.*, J. Chem. Phys. 158, 234103 (2023).

O 92.6 Thu 16:15 H25

**Enhancing structure relaxation with machine-learned interatomic potentials** — Sudarshan Vijay[1,2], Martijn Marsman[1], Georg Kresse[1,3], and •Martin Schlipf[1] — [1]VASP Software GmbH, Berggasse 21, 1090 Vienna, Austria — [2]Department of Chemical Engineering, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra 400076 India — [3]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Kolingasse 14-16, A-1090 Vienna, Austria

Machine learning interatomic potentials (MLIPs) offer a cost-effective way to predict ground-state properties of materials compared to density functional theory (DFT) calculations. MLIPs are often used to replace DFT due to their ability to access large length and longer time scales. In this study, we explore whether MLIPs can also enhance DFT by preconditioning commonly used optimization algorithms for structure relaxation. We demonstrate that applying this preconditioner to methods such as conjugate gradient (CG) and Broyden-Fletcher-Goldfarb-Shanno (BFGS) results in faster convergence but at the expense of stability. For this particular tasks, state-of-the-art MLIPs are not accurate enough to replace DFT; prerelaxing the structures with MLIPs tends to perform worse compared to starting the relaxation directly within DFT. Our analysis of the convergence behavior for both standard and preconditioned methods suggests that advancements in line-search techniques could enhance the effectiveness of this preconditioning approach for structure relaxation.

O 92.7 Thu 16:30 H25

**Constrained Density Functional Theory with Numeric Atomic Orbitals** — •Tavinder Singh[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology

Even in perfectly crystalline materials, simulation of some phenomena, such as the occurence and transport of polarons, rests on the simulation method's ability to describe localized charge carriers. This is generally hampered by both, the need to break a system's symmetry to accommodate such a localized state, and the infamous electron delocalization error of most semi-local density functionals. In this respect, constrained density functional theory (CDFT) has proven to be a viable tool addressing both. Constraining charges to pre-selected localized states naturally breaks the symmetry and mitigates DFT errors. In our contribution, we describe our implementation of CDFT in the FHI-aims package based on Numeric Atomic Orbital (NAOs) projectors. As a prototype, we consider polaron localization in the zero-strain anode material, $Li_4Ti_5O_{12}$ (LTO), and compared the computed relative energies and barriers with the literature as benchmark. Our results provide valuable insights into the applicability and accuracy of CDFT for studying localized electronic states in complex materials.

O 92.8 Thu 16:45 H25

**Efficient Phonon Dispersions of 2D Films by Extension of DFPT in FLAPW Method *FLEUR* to Film Geometry.** — •Thomas Bornhake[1,2], Alexander Neukirchen[1,2], Gregor Michalicek[1], Daniel Wortmann[1], Gustav Bihlmayer[1], and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Physics Department, RWTH Aachen University, Aachen, Germany

Phonons are crucial in 2D materials, governing a range of physical properties and phenomena, *e.g.* from dynamical stability to spin-flip scattering. Thus, an efficient method for calculating phonons under arbitrary excitations is inevitable. Typically, phonons of film systems are calculated from *ab initio* using supercells that separate the film from periodic images by computationally costly empty space. Recently, we have succeeded in calculating the phonon dispersion using the state of the art density functional perturbation theory (DFPT) in the all-electron full-potential linearized augmented planewave (FLAPW) method *FLEUR* [1,2]. In this talk we present our extension to a truly 2D treatment of films embedded in semi-infinite vacuum [3]. We discuss some details of the implementation and compare results with respect to accuracy and efficiency to the repeated slab approaches.

This work was supported by CoE-MaX (EuroHPC JU, Grant No. 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] H. Krakauer *et al.*, Phys. Rev. B **19**, 1706 (1979).

O 92.9 Thu 17:00 H25

**Excitations in oxides: from bits to qubits** — •Vijaya Begum-Hudde[1], Yi-Ting Lee[1], Barbara Jones[2], and Andre Schleife[1] — [1]University of Illinois, Urbana-Champaign, USA. — [2]IBM

Defects in materials are ubiquitous and may adversely affect their functional properties. Often the defects are confined to a small space, and defect embedding allows us to define an active space comprising of these defect states and to incorporate screening effects of the host material, enabling access to electronic properties with a high-level theory. In this talk I will focus on the structural and electronic properties of near-surface vacancies in $\alpha$-$Al_2O_3$ (0001) to investigate the influence of defects and hydration on the initiation and propagation of corrosion in this material. Utilizing first-principles calculations and quantum-defect embedding theory calculations, this study will analyse defect states and their ground- and excited-state properties. An active space is defined consisting of strongly localized states of the surface O vacany, and the remainder is treated as the environment. Next, an effective Hamiltonian is used for the active space that also includes the environment's effective screening and is solved via full configuration interaction (FCI). Simulations are performed on a quantum computer with a Unitary coupled-cluster ansatz for the determination of ground- and excited-state properties. Error mitigation techniques will be demonstrated, reducing error due to the hardware noise and showing very good concordance with the FCI results within chemical accuracy.

We acknowledge funding by the IBM-Illinois Discovery Accelerator Institute.

O 92.10 Thu 17:15 H25

**Electronic band structure at finite temperature: A unifying approach that incorporates electron-electron and electron-vibration interactions** — •Min-Ye Zhang[1,2], Xinguo Ren[2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft — [2]Institute of Physics, Chinese Academy of Sciences, China

An accurate first-principles description of electronic band structure at finite temperature requires accounting for self-energy contributions from both electron-electron (e-e) and electron-vibration (e-vib) interactions. In the widely used electron-phonon coupling (EPC) model[1], the two types of interactions are considered separately, and the model fails for strongly anharmonic materials. In this work, we integrate the two types of interactions beyond the EPC model by extending the statistically anharmonic, higher-order vibronic coupling approach[2] with the many-body $GW$ method. This is achieved by combining *ab initio* molecular dynamics and periodic $G^0W^0$ method in an all-electron framework employing numeric atom-centered orbitals[3]. We demonstrate the robustness and efficiency of our $G^0W^0$ implementation, particularly through a proper treatment of long-range dielectric responses. As a proof of concept, we present the temperature-dependent electronic band structure of Si, incorporating both e-e and e-vib interactions.

[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).
[2] M. Zacharias, M. Scheffler, and C. Carbogno, *Phys. Rev. B* **102**, 045126 (2020).
[3] X. Ren, et al, *Phys. Rev. Materials* **5**, 013807 (2021).

O 92.11 Thu 17:30 H25

**Electronic and optical properties of computationally predicted Na-K-Sb crystals** — •Chung Xu, Richard Schier, and Caterina Cocchi — University of Oldenburg

Due to their favorable electronic and optical properties, sodium-potassium-antimonides are an emerging class of crystals used as photocathodes in particle accelerators. Using first-principles methods based on density-functional theory and many-body perturbation theory, we investigate the electronic and optical properties of cubic $NaK_2Sb$ and hexagonal $Na_2KSb$, two computationally predicted polymorphs of established photocathode materials that can emerge as metastable phases in polycrystalline samples. Our results indicate that both systems are indirect band-gap semiconductors with fundamental gaps on the order of 0.7 and 0.8 eV, respectively. Their direct gaps are very close to these values and Their optical spectra are characterized by weakly bound excitons in the near-infrared region which represent favorable characteristics for efficient photoemission. Our study suggests that the presence of cubic $NaK_2Sb$ and hexagonal $Na_2KSb$ in photocathode samples is not detrimental for their application as photocathodes [1].

[1] arXiv:2411.13330

O 92.12 Thu 17:45 H25

**Thermal dependence of conductance in short pi-conjugated single-molecule junctions** — •Václav Kubíček and Hector Vazquez — Inst. of Physics, Czech Academy of Sciences

Conductance measurements at room temperature in single-molecule junctions are affected by the internal dynamics of the molecule, since many different internal conformations are averaged. Further temperature changes lead to different conformational sampling and may alter conductance values, opening the possibility of thermally active molecular devices.

For example, it was measured that raising the temperature from 300 K to 330 K results in a change in conductance for oligophenylenes [1]. In our work, we calculate the temperature dependence of conductance for several short pi-conjugated molecular wires. By combining classical statistical model with DFT simulations, we explore their accessible geometries and compute the resulting changes in conductance.

Our results show that by engineering chain composition, conductance increases or decreases are achievable with increasing temperature. Our results demonstrate the importance and potential applicability of thermally induced conformational changes in conductance.

[1] Lee, W.; et al., Nano Lett. 2022, 22, 4919

O 92.13 Thu 18:00 H25

**Comparison of non-equilibrium Green function and wave packet methods for studying the CISS effect** — •Thibaut Lacroix, Clemens Vittmann, Jaemin Lim, Susana F. Huelga, and Martin B. Plenio — Intitut für Theoretische Physik, Universität Ulm, Ulm, Deutschland

Non-equilibrium Green function (NEGF) technique has been widely employed to simulate quantum transport at the molecular scale. It is one of the main methods used to study transport properties of chiral molecules which are central to the investigation of chirality induced spin selectivity (CISS). Equivalent to the solution of a scattering problem, this approach leads to an energy resolved description of transport properties that can be used to obtained spin-dependent currents.

Alternatively, the description of electronic transport can be performed at the level of the Schrödinger equation. In that case, one considers an initial wave packet in the position basis – which therefore corresponds to a superposition of energy eigenstates – and computes its dynamics under the total Hamiltonian of the molecule and the leads. One benefit of this approach is to readily give access to the transient dynamics of the electron inside of the molecule, thus opening the possibility to study the internal mechanisms underlying CISS. We demonstrate that NEGF results can be recovered from wave packet evolution and that tailored wave packets enable to access directly specific transport properties of interest. These results show that while they rely on different formalisms wave packet evolution and NEGF do give the same information about the response of the system.

## O 93: Members' Assembly

Time: Thursday 19:00–19:30 Location: H1

**break**

## O 94: Post Deadline Session

Time: Thursday 19:30–20:30 Location: H1

# O 95: Overview Talk Kai Rossnagel

Time: Friday 9:30–10:15 Location: H24

**Topical Talk** O 95.1 Fri 9:30 H24

**A quantum sandwich world and how we can explore it with soft x-rays** — •Kai Rossnagel — Kiel University, Kiel, Germany — DESY, Hamburg, Germany

Without materials, there is nothing. Without quantum materials, there is nothing interesting.

Quantum materials express our desire to find and explain new states of matter and new physical phenomena induced by the quantum mechanical interactions of electrons. Paradigmatic examples are quantum material sandwiches made by stacking and twisting single layers of layered materials, which currently represent one of the richest and most tunable discovery and engineering platforms in all of condensed matter physics.

To see and understand how these and other quantum materials work, we need spectroscopic tools that can provide direct snapshots of electron behavior in energy-momentum space. The most powerful toolbox for this is soft x-ray spectroscopy. And the single most powerful tool is angle-resolved photoelectron spectroscopy (ARPES), which has recently been transformed into a true *in operando* technique using both nanofocused and ultrashort-pulsed soft x-ray beams to directly probe nonequilibrium electronic function in materials and devices on relevant nanometer length and femtosecond time scales, respectively.

Here, we give an overview of recent innovations in quantum material sandwiches, focusing on transition-metal dichalcogenides, and in nanoscopic and femtostroboscopic imaging of their electronic structures.

# O 96: Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy II

Time: Friday 10:30–13:00 Location: H4

O 96.1 Fri 10:30 H4

**Enhancing light-matter interaction through inverse design of optical devices.** — •Carlos Bustamante[1], Mark Svendsen[2], Franco Bonafé[1], Burak Gurlek[1], Maxim Sukharev[3], Abraham Nitzan[4], and Angel Rubio[1] — [1]MPSD, Hamburg, Germany — [2]Niels Bohr Institute, University of Copenhagen, Denmark — [3]Department of Physics, Arizona State University, USA — [4]Department of Chemistry, University of Pennsylvania, USA

Light-matter interaction plays a crucial role in processes such as spontaneous emission, energy transfer and polaritonic formation. This interaction is sensitive to alterations in the electromagnetic environment which can be caused by the presence of optical materials. In classical optics, changes in the topology of optical materials can lead to the fabrication of optical devices tailored towards specific characteristics, using inverse design methodologies like density-based topology optimization (TO). This work presents the application of optical devices, derived from TO, that can be used to modify light-matter interaction among molecules. To achieve this, we have implemented a TO algorithm that can solve Maxwell equations in the frequency domain on a 2D grid. These tailored devices enhance locally one component of the transverse electric field obtained from classical emitters. In subsequent semiclassical simulations, Maxwell equations were classically propagated with the emitters replaced by pentacene molecules using the quantum mechanical simulation software DFTB+. The results highlight the significant potential of optical devices produced by TO to influence the above-mentioned processes.

O 96.2 Fri 10:45 H4

**Squeezing few-cycle light pulses in space and time in the gap of a nanoplasmonic resonator** — •Tom Jehle, Sam S. Nochowitz, Juanmei Duan, and Christoph Lienau — Universität Oldenburg, D-26129, Germany

The spatial confinement of light to (sub-)nanometer spot sizes in the gap of a nanoparticle-on-mirror resonator or in the gap of a tunnelling junction has led to dramatic advances in nanosensing [1] and tip-enhanced Raman Spectroscopy [2]. So far, the time dynamics of the fields emitted from such nanocavities have achieved little attention and only recently the time structure of a Terahertz field scattered from the junction of an STM tip could be recorded [3]. Here, we introduce a broadband interferometric scattering-type SNOM technique [4] to reconstruct amplitude and phase of light scattered from a sharp gold taper acting as a near-field probe. Direct Fourier transform gives the time structure of the electric field. We distinguish the near-field scattered from the apex and that emitted by spatially well separated scattering mode of the taper. The apex field decays within 13 fs, a decay time mainly given by the radiative damping of the apex mode. Upon approaching the tip to a gold surface, we observe a 3.5-fold reduction in the decay time to less than 4 fs: coupling to the image dipole drastically increases the radiative damping in the tip-surface junction. 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] R. Zhang et al., Nature 531, 623 (2016); [3] T. Siday et al., Nature 629 (2024); [4] J. Zhan et al., Nano Lett. 2024

O 96.3 Fri 11:00 H4

**Full-wave simulations of core-shell nanoparticle investigation by tapping mode near-field optical microscopy** — •Dario Siebenkotten, Dinghe Dai, Richard Ciesielski, Arne Hoehl, and Bernd Kästner — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12 10587 Berlin

Core-shell nanoparticles are important in applications such as optoelectronics, biosensing, and medicine, where their unique optical and geometric properties play a critical role in functionality. Quantifying the properties of both, the core and the shell, is crucial to understand the nanoparticle's ultimate functionality. However, optical investigation of their properties, while widely employed, is generally diffraction-limited and thus unsuitable for the investigation of individual nanoparticles, as they only provide averaged ensemble information. Scattering-type scanning near-field optical microscopy (s-SNOM) promises access to a single nanoparticle's size and optical properties through the use of an atomic force microscopy tip as an optical antenna, which confines the sampling fields to nanoscale dimensions. To explore the single nanoparticle s-SNOM response, we model different core-shell nanoparticles using Finite Element Modelling, revealing complex resonance-antiresonance behaviour in dependence of their geometrical and optical properties. We further explore the origin of the emergent antiresonance through the use of Fourier-demodulation of the probe tapping [1], closely mimicking the experiment. [1] Mooshammer et al., ACS Photonics 7, 344-351 (2020)

O 96.4 Fri 11:15 H4

**Near-field microscopy of complex polaritonic excitations** — •Farid Aghashirinov[1], Bettina Frank[1], Harald Giessen[1], Andrea Manchini[2], Lin Nan[2], Giacomo Venturi[2], Nicola Melchioni[2], and Antonio Ambrosio[2] — [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 (NIR) plasmon polaritons (PPs) in mechanically exfoliated bulk molybdenum oxide dichloride (MoOCl2) flakes on a glass substrate with gold disk launchers positioned on top of the flakes, through experimental and theoretical methods [1]. MoOCl2, a natural van der Waals crystal, exhibits low-loss, in-plane hyperbolic PPs across the visible and NIR ranges, and displays a unique anisotropic optical response based on the polarization of the incident light. When light polarization aligns with the flake's shortest axis, MoOCl2 behaves optically metallic, while aligning with the longest axis reveals a dielectric behaviour. To experimentally study the hyperbolic PPs in MoOCl2, we use a near-field excitation and detection approach. Gold disks serve as excitation sources, scattering incident light to couple it with the material's polaritonic modes, while a reflection scattering-type scanning near-field optical microscope (s-SNOM) enables subwavelength imaging. For tunable wavelength illumination, we use a broadband laser from Stuttgart Instruments (SI), which, when combined with s-SNOM, allows us to investigate these modes across a wide wavelength range, capturing detailed insights into their behavior and propagation. [1] G. Venturi et al., Nat Commun 15, 9727 (2024)

O 96.5 Fri 11:30 H4

**Discovery of phonon-polaritonic skyrmions: Transition from bubble- to Néel-type** — •Florian Mangold[1], Enrico Baù[2], Lin Nan[2], Julian Schwab[1], Thorsten Gölz[2], Andrea Mancini[2], Bettina Frank[1], Andreas Tittl[2], and Harald Giessen[1] — [1]4th Physics Institute, Research Center SCoPE, and IQST, University of Stuttgart, Germany — [2]Chair in Hybrid Nanosystems, Nano-Institute Munich, Ludwig-Maximilians Universität München, Germany

Optical skyrmions constitute an emerging and rapidly developing field in the domain of solid-state physics and photonics, allowing for control over topological light textures through light-matter interactions. However, until now their practical applications have been severely limited by inherent restrictions of materials with high optical losses and a lack of tunability between different topological properties. We leverage the steep dispersion of silicon carbide thin films to image surface phonon polariton skyrmion lattices via near-field microscopy and experimentally demonstrate topological tuning between Bubble- and Néel-type skyrmions, a unique advantage that polar dielectrics offer over most existing approaches. The ability to control and manipulate these skyrmion lattices through small changes (<10%) in excitation wavelength allows for tailoring the size of individual skyrmions by a factor of 4. Tuning topological properties has been a long-standing goal in the field of optics. Our results expand the tunability of skyrmions in evanescent waves and are a starting point to investigate other topological features in phononic systems such as merons, skyrmion bags and other complex structured light fields.

O 96.6 Fri 11:45 H4

**Tracking Non-Equilibrium Electron Distributions to Propel Chemical Dynamics at Surfaces** — •Henry T. Snowden[1], Reinhard J. Maurer[1], Markus Uehlein[2], and Baerbel Rethfeld[2] — [1]University of Warwick, Coventry, UK — [2]RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

A mechanistic understanding of ultrafast light-matter interactions with surfaces and nanoparticles is invaluable for the study of ultrafast dynamics at surfaces. Immediately after a laser pulse, non-equilibrium electrons are generated in metals which rapidly relax to a thermal distribution that follows the two-temperature model. Here, we study the longevity of electronic non-equilibrium which depends on the electronic structure and other materials properties. We simulate the temporal evolution of non-equilibrium electron distributions with the Athermal Electron Model (AthEM), which explicitly considers electronic nonequilibrium, a laser term and electron scattering in the relaxation time approximation. Equipped with this approach, we investigate how athermal electron-hole pair distributions differ in various materials configurations such as intermetallic interphases, and nanoparticles. We will use this information to discuss the requirements to create long-lived non-equilibrium distributions from which high-energy charge carriers can be harvested.

O 96.7 Fri 12:00 H4

**Collective Behavior of SiC Phonon Polariton Resonators** — •Richarda Niemann[1,2], Sören Wasserroth[1], Guanyu Lu[2], Christopher R. Gubbin[3], Martin Wolf[1], Simone de Liberato[3], Joshua D. Caldwell[2], and Alexander Paarmann[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]Vanderbilt University, Nashville, TN, USA — [3]University of Southampton, Southampton, UK

Structuring polar materials with microresonators enables light confinement to sub-wavelength scales and the emergence of localized phonon polaritons (PhPs). Previous studies on PhP single resonators and 2D resonator arrays investigated the coupling behavior of resonators with their surrounding [1,2]. Here, we bridge the gap between a single resonator and a 2D array by studying subdiffractional SiC microresonators on a SiC substrate in 1D arrays with sumfrequency generation (SFG) spectro-microscopy [3,4]. The high spatial resolution on the order of the lateral size of the microresonators allows us an in-depth analysis of the build-up of collective modes in 1D arrays with sizes from one to several resonators. We observe different optical responses for in-phase and out-of-phase excitation showing the importance of phase relationships for coupling between the resonators. By investigating arrays with different periods, we gain information about the coupling mechanisms.

[1] Gubbin et al., Phys. Rev. B, 95 (2017)
[2] Chen et al., ACS Photonics, 1 (2014)
[3] Niemann et al., Appl. Phys. Lett. 120, 131102 (2022)
[4] Niemann et al., Adv. Mater. 2024, 36, 2312507

O 96.8 Fri 12:15 H4

**High-Throughput 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]University of 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]. However, little is still known about the trends in material space that drive the emergence and characteristics of PhPs. To describe these trends, we compute the permittivity function [2] as the basis for describing PhP dispersion. We employ Kubo's linear-response theory, where the harmonic and anharmonic phonon properties as well as Born effective charges are used to model the involved couplings. This approach is validated on materials with well-characterised PhP behaviour, such as h-BN, MoO$_3$ and $\beta$-Ga$_2$O$_3$, and then applied to 5,000 materials from the JARVIS database [3]. By analysing the trends emerging from these data, we identify qualitative metrics that capture the material's ability to support PhPs. Finally, we highlight some examples and outliers of this high-throughput screening process.

[1] E. Galiffi *et al.*, *Nat. Rev. Mater.* **9**, 9 (2024).
[2] M. Born & K. Huang, *Dynamical Theory of Crystal Lattices* (1954).
[3] K. Choudhary *et al.*, *npj Comput. Mater.* **6**, 1 (2020).

O 96.9 Fri 12:30 H4

**Electron Relaxation in Noble Metals: Microscopic Theory of Orientational Relaxation, Thermalization and Cooling** — •Jonas Grumm and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany

The excitation of electrons in noble metals by light fields with high intensities results in non-equilibrium electron occupations. The relaxation back to thermodynamic equilibrium, proceeding on scales from a few femtoseconds to several picoseconds, depends strongly on these excitation conditions: Typically, during the first tens of femtoseconds after the excitation, momentum polarization induced by the distinct polarization direction of the light field dominates the electron gas.

To address the relaxation dynamics of this momentum polarized state, we solve a kinetic momentum-resolved Boltzmann equation with focus on electron-phonon interaction and introduce orientational relaxation as first temporal step in a sequence of relaxation processes followed by thermalization and cooling. Applying a self-consistent treatment of Maxwell's equations and material dynamics we are able to present results for the optical and thermal properties of plasmonic nanostructures after linear and non-linear optical excitations. Thereby, Pauli-blocking non-linearities in the electron-phonon interaction modify the relaxation dynamics for strong excitations and effect the optical response of the electron gas.

O 96.10 Fri 12:45 H4

**Sum-Frequency Generation Spectro-Microscopy in Barium Titante** — •Dorothee Mader[1], David Pesquera[2], Saptam Ganguly[2], Richarda Niemann[1,3], Martin Wolf[1], Sebastian F. Maehrlein[1], Jose Santiso[2], and Alexander Paarmann[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain — [3]Vanderbilt University, Nashville, USA

Ferroelectric Barum Titanate (BTO) can be switched by excitation of phonons in the infrared (IR), enabeling the applications in future optical technologies.[1] Here, we investigate the resonance behavior of BTO in the IR by employing infrared-visible (IR-VIS) sum-frequency generation (SFG) spectro-microscopy using the free-electron laser of the Fritz Haber Institute.[2,3] As a second-order nonlinear technique, this method is sensitive to the material's symmetry. Additionally, as it is employed resonantly, it can reveal vibrations, local structure and bonding of the material. We demonstrate resonant ferroelectric imaging using SFG spectro-microscopy for bulk BTO and 500 nm thin BTO membranes.

[1] M. Kwaaitaal et al., Nat. Photonics 82(3), 2731, (2024).
[2] R. Niemann et al., Appl. Phys. Lett. 120, 131102, (2022).
[3] D. Mader et al., J. Chem. Phys. 161, 094706 (2024).

# O 97: Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties II

Time: Friday 10:30–12:30 Location: H6

O 97.1 Fri 10:30 H6

**Nanostructuring of organic radicals on hybrid interfaces** — •Arkaprava Das, Ewa Malgorzata Nowik-Boltyk, Tobias Junghoefer, and Maria Benedetta Casu — Institute of Physical and Theoretical Chemistry, University of Tübingen, 72076 Tübingen, Germany

Organic radicals are potential candidates for groundbreaking applications like energy storage, quantum computing, and spintronics. In order to investigate the nature of the adsorption of the radical derivative molecules on hybrid surfaces based on polycrystalline Au and native $SiO_2$, 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 substrate-dependent 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.

O 97.2 Fri 10:45 H6

**Beyond the Koopmans' theorem: Energy-level alignment of PTCDA on BlueP-Au-network on Au(111)** — •Maximilian Schaal[1], Felix Otto[1], Marco Gruenewald[1], Roman Forker[1], Keisuke Fukutani[2], Satoshi Kera[2], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan

Koopmans' theorem is often used to relate the observed spectroscopic features in UP spectra to the orbital energies of molecules calculated by Hartree-Fock calculations. However, this theorem neglects the self-energy (charging energy), which can be as large as 1 eV for molecules in the gas phase [1]. Therefore, the ground state energy levels of the frontier orbitals are not sufficient to describe the energy-level alignment and the initial and final states must be considered [2].

In this study, we present a framework to investigate the energy-level alignment of a monolayer of PTCDA decoupled from the Au(111) surface by a BlueP-Au-network [3]. We have determined the electronic transport and the optical gap using differential reflectance and (low-energy inverse) photoelectron spectroscopy. From these values, we determined the exciton binding energy and the charging energy. Finally, we compared the energy levels of the adsorbed monolayer with measured and calculated quantities of molecules in the gas phase.

[1] Kirchhuebel *et al.*, J. Phys. Chem. C **124** (2020).
[2] Kirchhuebel *et al.*, Phys. Chem. Chem. Phys. **21** (2019).
[3] Gruenewald *et al.*, Phys. Rev. Materials **6** (2022)

O 97.3 Fri 11:00 H6

**Disentangling the components of a multireference excited state in an isolated chromophore** — Rodrigo Ferreira[1,2], Tomáš Neuman[1], Amandeep Sagwal[1], Jiří Doležal[2], Petr Kahan[1], and •Martin Švec[1,2] — [1]Institute of Physics, Czech Academy of Sciences — [2]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

Excited states of open-shell chromophores are commonly multireference in their nature. Distinguishing the components of these superposition states in a single chromophore by experimental means is a challenging task as it would essentially require capturing their orbital occupancies in the excited state. We demonstrate this can be achieved by atomically precise mapping of photon-induced tunneling current under a varying electric field, on a model case of a PTCDA anionic excited state coupled to a plasmonic nanocavity. To simulate the cascade of energy conversions and charge transfer events occurring within the molecule, a set of rate equations is derived from a many-body state scheme using an input from TD-DFT. The resulting bias-dependent tunneling current maps reach a very good agreement with the experimental data, corroborating the validity of the theoretical understanding.

O 97.4 Fri 11:15 H6

**Second harmonic spectroscopy of Fe-porphyrin/Cu(001) interfaces** — •Newsha Vesalimahmoud, Mahendra Kabbinahithlu, Ping Zhou, Uwe Bovensiepen, and Andrea Eschenlohr — University of Duisburg-Essen, Faculty of Physics and CENIDE, Lotharstr. 1, 47057 Duisburg, Germany

When a molecule interacts with a metal surface, metal-molecule interaction induces a rearrangement of their electronic densities, shifting the molecular orbitals relative to the metal's Fermi level. This study focuses on the FeOEP/Cu(001) interface, using interface-sensitive SHG spectroscopy. We analyze polarization- and wavelength-dependent SHG for varying molecular adsorbate thicknesses on Cu(001) using a fundamental beam in the 500-600 nm range. Polarization-dependent measurements show a higher SHG yield for p-P polarization than s-P SHG, as the intrinsic value of $\left|\chi^{(2)}_{zzz}\right|$ is much larger than $\left|\chi^{(2)}_{zxx}\right|$. As the number of monolayers increases, P-polarized SHG intensity decreases due to reduced nonlinear susceptibility from less polarizable free electrons, while S-polarized SHG shifts from 4-fold to 2-fold symmetry. The SHG spectra show an intensity peak at 2.17 eV due to a one $\omega$ resonance in Cu(001). After adsorption of 2, 5, and 8 monolayers (ML) of FeOEP on Cu(001), the spectral dependence remains similar to the Cu(001) surface, except for an enhancement at 2.21 eV for 5ML and 8ML. This enhancement is attributed to the energetic position of the lowest unoccupied molecular orbital (LUMO) at the FeOEP/Cu(001) interface.

O 97.5 Fri 11:30 H6

**Probing the Roles of the Substrate Material, Spin Scattering, Temperature and Cooperative Effects in CISS** — •Paul V. Möllers[1], Adrian J. Urban[2,3], Bianca C. Baciu[4], Rafael Rodriguez[5], Albert Guijarro[4], Jeanne Crassous[5], Steven De Feyter[3], Hiroshi M. Yamamoto[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience (SoN), University of Münster, Busso-Peus-Str. 10, 48149 Münster, Germany — [2]Institute for Molecular Science, Research Center of Integrative Molecular Systems, Division of Functional Molecular Systems, 38 Nishigonaka, Myodaiji Okazaki, Aichi prefecture, 444-8585 Japan — [3]Division of Molecular Imaging and Photonics, Department of Chemistry, KU Leuven, Celestijnenlaan 200 F, 3001 Leuven, Belgium — [4]Departamento de Química Orgánica, Instituto Universitario de Síntesis Orgánica, Unidad asociada al CSIC, Universidad de Alicante, E-03080, Alicante, Spain — [5]University of Rennes, CNRS, Institut des Sciences Chimiques de Rennes (ISCR), UMR 6226, Rennes, France

Monolayers of heptahelicene ([7]H) and helical tetrapyrrole (TPBT) complexes were adsorbed onto different single-crystalline metal substrates, and the spin polarization of photoelectrons emitted from these surfaces was measured. The substrate material, the temperature and the surface coverage were systematically varied to investigate the roles of the substrate spin–orbit coupling, molecular vibrations, and intermolecular interactions in the generation of the spin polarization. Furthermore, thiolized (chemisorbed) [7]H and all-carbon (physisorbed) [7]H layers were compared.

O 97.6 Fri 11:45 H6

**Electrons don't wear bowties: The mechanism of Fermi-level pinning and charge for mixed donor-acceptor layers** — •Richard Berger1 and Oliver T. Hofmann — TU Graz, Institute of Solid State Physics

Controlling the work function of metal substrates is critical when optimizing the performance of organic electronic devices. A particular powerful method to obtain such control is by employing a monolayer of strong electron donors or electron acceptors, i.e. so-called Fermi-level pinned systems which form charge-transfer-induced dipoles with the underlying substrate However, while the major advantage of this Fermi-level pinned systems is that the effective work function of the interface is (essentially) independent of the underlying substrate, there are only limited ways to fine-tune it. A more flexible way could be to employ a mixture of electron donors and acceptors. However, for such complex systems the underlying charge-transfer mechanism is less clear. In this work, we elucidate this mechanism using machine-learning augmented density functional theory calculations to predict both the atomistic and the electronic structure of the interface using a mixture of F4TCNQ and paraquat as an example. Counterintuitively, we find that the nominally weaker donor overpowers the stronger acceptor, resulting in a dependence of the work function that is effectively determined by the nominal coverage of the donor. At the same time, we find that multiple geometries are energetically very similar, but result in different work function, affecting the reproducibility of different experimental realizations.

O 97.7 Fri 12:00 H6

**Magnetic Coupling in Triangulene Dimers: Impact of Number and Dihedral Angles of para-Biphenyl Linkers** — •Marco Lozano[1], Elena Perez-Elvira[2], Qiang Huang[3], Ji Ma[3], Aurelio Gallardo[2], Ana Barragan[2], Alba Garcia-Frutos[2], Koen Lauwaet[2], Jose Gallego[4], Pavel Jelinek[1], David Ecija[2], Diego Soler-Polo[1], and Jose Urgel[2] — [1]Institute of Physics of the Czech Academy of Science, CZ-16253 Praha, Czech Republic — [2]IMDEA Nanoscience, C/ Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain — [3]Center for Advancing Electronics Dresden (cfaed) & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01069 Dresden, Germany — [4]Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC, Cantoblanco, 28049 Madrid, Spain

Triangulene and its homologues are promising building blocks for high-spin low-dimensional networks with long-range magnetic order. Despite the recent progress in the synthesis and characterization of coupled triangulenes, key parameters such as the number or the dihedral angles of organic linking units remain scarce, making further studies crucial for an essential understanding of their implications. Here, we investigate the synthesis of two triangulene dimers linked by two or one para-biphenyl units on a metal surface in an UHV environment. First-principles calculations and model Hamiltonians reveal how the spin excitation and radicalism depend on the rotation of the para-biphenyl units.

O 97.8 Fri 12:15 H6

**Insights into Nonlinear CD-ee Dependence in Tryptophan Thin Films** — •Charitini Panagiotopoulou, Changseop Jeong, Ueli Heiz, and Aras Kartouzian — Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Chiral analysis is essential, especially for enantio-separation and -enrichment, with Circular Dichroism (CD) spectroscopy being a fast and straightforward method for studying enantiomeric excess (ee) and its dependence on circular dichroism (CD-ee dependence). While most systems show linear CD-ee dependence, studies reporting non-linear CD-ee behaviour are relatively rare and, thus, more attractive for research. Building on our earliest findings of negative nonlinear CD-ee dependence in polycrystalline BINOL thin films (Liang et al. 2023), we extend this study to a different system: the well-known amino acid responsible for synthesizing important proteins in humans, Tryptophan. We prove our hypothesis that the non-linear CD-ee dependence is not limited to BINOL films and can be applied to biomolecules, and we outline this non-linear dependence with different methods, such as CD spectroscopy, SHG-CD spectroscopy and FTIR study. This behaviour is linked to the structural characteristics of Tryptophan when a series of different enantiomeric excesses are deposited onto thin films via molecular evaporation. This approach paves the way for extensive exploration in the field of biomolecular chirality.

## O 98: Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules

Time: Friday 10:30–12:30 Location: H8

O 98.1 Fri 10:30 H8

**Bonding properties of a CO molecule with metallic adatoms** — •Fabian Stilp, Marco Weiss, Maximilian Krüger, and Franz J. Giessibl — Department of Physics, University of Regensburg

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 as evident by an attractive center within a repulsive ring in constant height AFM measurement. 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 on various adatoms by adding Ni and Ag.

Ni has a partially filled d-shell and thus forms a chemical bond of similar strength as Fe. Surprisingly, Ag with its similar electron configuration as Cu, immediately goes to Pauli repulsion while Cu first forms a weak bond.

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

O 98.2 Fri 10:45 H8

**Adsorption sites of merocyanines on the Ag(100) surface determined by NIXSW** — •Anna Juliana Kny[1], Anja Haags[2], Sergey Subach[2], and Moritz Sokolowski[1] — [1]Clausius Institut für Physikalische und Theoretische Chemie, Universität Bonn, Germany — [2]Forschungszentrum Jülich, Germany

The growth of thin organic layers is strongly influenced by the interactions between the molecule and the substrate surface. We report about the adsorption sites of a series of merocyanine (MC) molecules on the Ag(100) surface. MCs are prochiral donor-acceptor molecules which are in focus for applications due to high transition dipole moments. [1] Remarkably, SPA-LEED data reveal commensurate structures for all of our investigated MCs, although the size of the unit cells depends on the length of the alkyl side chains.[2] In order to answer the question of what is behind the commensurate growth of these complex molecules, we performed an XPS and an NIXSW investigation. We find a strong binding of the two sulfur heteroatoms, located in the thiophene and the thiazole rings, to the Ag surface. This can be seen in charge transfer and an adsorption of the S-atoms close to on-top sites. This is found for all investigated structures. Furthermore, compatible with the symmetry of the unit cell, the results reveal that the four molecules per unit cell sit on two different adsorption sites.

We acknowledge experimental support from D.A. Duncan (DLS). Supported by the DFG through the research training group 2591 and the Diamond Light Source, UK.

[1] JACS 137 (2015) 13524. [2] Nanoscale 15 (2023) 10319.

O 98.3 Fri 11:00 H8

**Electron-Induced Dehydrogenation of Acetylene and Ethylene on Si(100)** — Rafik Addou, Damian Allis, Ryan Groome, Si Yue Guo, Aru Hill, Hadiya Ma, Cameron Mackie, •Oliver MacLean, Marc Savoie, Marco Taucer, Alexander Therien, Finley van Barr, and Ryan Yamachika — CBN Nanotechnologies Inc.

Low-Temperature Scanning Tunneling Microscopy (STM) is a powerful tool for manipulating individual atoms and molecules on surfaces. The Si(100) surface is a technologically relevant substrate; however, its high reactivity and structural complexity has led to limited examples of molecular manipulation. Here, we demonstrate the electron-induced dehydrogenation of two simple hydrocarbons on Si(100) at 4 K. Excitation by tunneling electrons at or above +3.2 V led to rotation, migration, or desorption of acetylene, consistent with previous observations on ethylene. At similar biases, dehydrogenation to C2 was also observed, which bound in on-dimer, inter-dimer, and inter-row configurations, as supported by STM simulations. At +4.2 V and above, excitation induced rotation of C2 between configurations, but conversion back to the starting adsorbates was never observed. Tunneling-electron excitation of ethylene yielded the same C2 products. Dehydrogenation of acetylene by field emission was also observed, with an effect ranging from a single to thousands of molecules, depending on the parameters chosen. This exploration of electron-induced dehydrogenation and rotation points to new possibilities in molecular manipulation on semiconductors.

O 98.4 Fri 11:15 H8

**Selectivity on and off: adsorption of allyl ethers on Si(001)** — •Sophie Göbel[1], Timo Glaser[1], Alexa Adamkiewicz[2], Jannick Peters[1], Julian Heep[1], Ulrich Höfer[2], and Michael Dürr[1] — [1]Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Fachbereich Physik, Philipps-Universität Marburg, Germany

Adsorption of organic molecules with more than one functional group on solid surfaces is of importance in the field of molecular electronics as they can be the starting point for multilayer systems [1]. To obtain well-organized monolayers of such bifunctional molecules, the understanding of their adsorption behavior, in particular in terms of their selectivity, is mandatory.

For allyl methyl ether (AME) and allyl ethyl ether (AEE), which combine an ether group with a C=C double bond, we show by means of XPS and STM that the adsorption of these molecules on Si(001) proceeds selectively via ether cleavage up to room temperature. The results are surprising as both functional groups involved show in general high reactivity on Si(001) and the ether group is less reactive when the isolated functional groups are compared. In contrast to AME and AEE, no such selectivity was observed for methoxy butene, where both functional groups are separated by an additional $CH_2$ unit. The results are discussed in terms of the interplay of electronic and geometric structure and its influence on the adsorption process.

[1] T. Glaser, et al., Chem. Mater. 36, 561 (2024).

O 98.5 Fri 11:30 H8

### The Effect of Doping in Inelastic H Atom Scattering from Silicon

— •Malte Opfermann, Sophia Tödter, Kerstin Krüger, and Oliver Bünermann — Institut für physikalische Chemie, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Recent inelastic H atom scattering experiments from the semiconducting Ge(111)c(2x8) have shown a bimodal energy loss distribution. One of the components was narrow with a small energy loss. The other component has shown a broad and large energy loss with an onset equal to the surface band gap.[1] While the low energy loss channel is explained by an adiabatic molecular dynamics simulation, the high energy loss component is not described theoretically yet.

To gain a better understanding of the underlying mechanism, we extended our studies to the Si(100)2x1 surface which is semiconducting as well. Despite its electronic structure being similar to the Ge(111)c(2x8) surface, it shows a different H atom energy-loss distribution. The first component is much broader and the second component does not show a clear onset at the surface band gap, both indicators of electronic effects. To further investigate, we carried out scattering experiments from samples with various doping levels.

[1] Krüger et al., Nat. Chem., DOI:10.1038/s,41557-022-01085-x (2022)

O 98.6 Fri 11:45 H8

### Adsorption and bowl inversion of sumenene adsorbed on Au(111): a density functional theory

— •Ikutaro Hamada[1], Ranmaru Kuno[1], Kota Iwata[2], Yoshiaki Sugimoto[2], and Hidehiro Sakurai[3] — [1]Department of Precision Engineering, Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan — [2]Department of Advanced Materials Science, The University of Tokyo, Kashiwa, Chiba 277-8561, Japan — [3]Division of Applied Chemistry, Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan

Sumanene, a bowl-shaped $\pi$-conjugated compound, has been shown to form an ordered overlayer on noble metal surfaces. It has also been shown to exhibit conformation change, namely, bowl inversion, depending on its environment [1,2]. Experimentally, we have found that on Au(111), sumanene forms an ordered overlayer that differs from the previously reported structure for Au(111), but resembles the one observed on Ag(111). Moreover, we have demonstrated that bowl inversion can be induced using an atomic force microscopy tip. In this work, we employ van der Waals density functional to investigate the geometric and electronic structure of sumanene on Au(111). We also investigate the detailed mechanism of the bowl inversion of sumanene within the overlayer on the surface.

[1] R. Jaafar et al., J. Am. Chem. Soc. 136, 13666 (2014). [2] S. Fujii et al., J. Am. Chem. Soc. 138, 12142 (2016).

O 98.7 Fri 12:00 H8

### Enhancing the electronic-coupling and conductivity of monolayer film of ferrocenyl molecules by Pd and Cu doping

— •Sunny M P Gautam, Himani Malik, Vikash Meghwal, Sruthi Manoharan, Vinithra Gurunarayanan, Ramesh Ramapanicker, and Thiruvancheril G Gopakumar — Department of Chemistry, Indian Institute of Technology Kanpur, India

Enhancing the conductivity and tuning the electronic structure of molecular films is crucial for their application in electronics. In this study, we explore the impact of metal doping (Pd and Cu) on the electronic structure and conductivity of two custom-designed ferrocenyl molecules, 3-ferrocenyl propanoic acid (FcC3) and 5-ferrocenyl pentadienoic acid (FcC5), on a graphite surface. Although the microscopic arrangement of the molecules within the film remains largely unchanged after doping, the incorporation of Pd and Cu at the 4-coordinated carboxyl dimer site of FcC3/FcC5 leads to a significant increase in conductivity. Electronic structure calculations of the FcC3/FcC5 dimers with metal show a substantial reduction in the HOMO-LUMO gap compared to their hydrogen-bonded counterparts, indicating stronger intermolecular electronic coupling through the Pd and Cu atoms, which lowers the barrier for electron/hole transport.

O 98.8 Fri 12:15 H8

### Ge(CH2I)4 on Si(100) - Matching the Molecule to the Surface

— •Brandon Blue, Rafik Addou, Damian G. Allis, Eduardo Barrera-Ramirez, Jeremy Barton, Adam Bottomley, Nina Cullum, Michael Drew, Tyler Enright, Alan Godfrey, Ryan Groome, Aru Hill, Taleana Huff, Robert J. Kirby, Samuel Lilak, Cameron J. Mackie, Oliver MacLean, Terry McCallum, Mathieu Morin, Matthew Moses, Jonathan Myall, Ryan Plumadore, Adam Powell, Henry Rodriguez, Marc Savoie, Benjamin Scheffel, Marco Taucer, Denis Alexander Therien, Dusan Vobornik, and Janice Wong — CBN Nanotechnologies Inc.

We present an on-surface, multi-technique analysis of a synthetic, custom molecule for Si(100): tetrakis(iodomethyl)germane - Ge(CH2I)4, or TIMe-Ge. TIMe-Ge consists of four iodomethyl (CH2I) legs bound to a Ge atom core in a tetrahedral geometry. TIMe-Ge was selected based on its expected reactivity and surface behavior with Si(100)-2x1 as part of a set of design criteria which we'll present and discuss. The suitability of TIMe-Ge with respect to these criteria were supported by simulations and literature precedent. TIMe-Ge was found to covalently bond with Si(100)-2x1 in a limited number of configurations via C-I dissociative addition by STM, DFT, and XPS. The fourth CH2I is oriented away from the surface and towards the SPM for interaction, including controlled generation of C-centered radicals via bias pulses and UV photochemistry. We anticipate that TIMe-Ge and its congeners will aid in the development of molecular nanotechnologies and the study of requisite intermediates.

# O 99: Ultrafast Electron Dynamics IV

Time: Friday 10:30–13:00 Location: H11

O 99.1 Fri 10:30 H11

**Large-amplitude coherent phonon dynamics in a van der Waals ferroelectric** — •Jan Gerrit Horstmann[1], Quintin Meier[2], Thomas Lottermoser[1], and Manfred Fiebig[1] — [1]Dept. of Materials, ETH Zurich, Switzerland — [2]Institut Néel, CNRS UPR2940, Grenoble, France

We explore the all-optical control of coherent phonon dynamics in the van der Waals ferroelectric $WTe_2$. Double-pulse optical excitation is harnessed to enhance the amplitude of the prominent interlayer shear mode beyond the limit of single-pulse excitation, with the resulting structural dynamics monitored via time-resolved second harmonic generation. A strong correlation between shear phonon amplitude and damping suggests higher-order coupling to lower-lying modes. At largest initial phonon amplitudes, Fourier transforms of the delay-dependent SHG traces reveal a frequency contribution at twice the shear-mode frequency. We discuss second-harmonic phonon generation and ultrafast phononic modulation of the nonlinear susceptibility as potential underlying mechanisms. Coherent vibrational control over relaxation pathways and electronic properties of ferroic van der Waals materials could enable novel types of devices for energy-efficient electronics.

O 99.2 Fri 10:45 H11

**Giant acceleration of polaron transport by ultrafast laser-induced coherent phonon** — •Huimin Wang[1,2], Xinbao Liu[1,2], Shiqi Hu[1,2], Daqiang Chen[1,2], Qing Chen[1,2], Cui Zhang[1,3], Mengxue Guan[1,2], and Sheng Meng[1,2,3] — [1]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China. — [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China. — [3]Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China

Polaron formation is ubiquitous in polarized materials, but severely hampers carrier transport for which effective controlling methods are urgently needed. Here, we show that laser-controlled coherent phonon excitation enables orders of magnitude enhancement of carrier mobility via accelerating polaron transport in a prototypical material, lithium peroxide (Li2O2). The selective excitation of specific phonon modes, whose vibrational pattern directly overlap with the polaronic lattice deformation, can remarkably reduce the energy barrier for polaron hopping. The strong nonadiabatic couplings between the electronic and ionic subsystem play a key role in triggering the migration of polarons, via promoting phonon-phonon scattering within subpicoseconds. These results extend our understanding of polaron transport dynamics to the non-equilibrium regime and allow for optoelectronic devices with ultrahigh on-off ratio and ultrafast responsibility, competitive with those of state-of-the-art devices fabricated based on free electron transport. H.M.Wang et al. Sci.Adv.9,eadg3833(2023).

O 99.3 Fri 11:00 H11

**Ultrafast charge density wave, Van Hove singularity and flat-band dynamics in the Kagome metal $CsV_3Sb_5$** — •Mohamed Amine Wahada[1], Chris Nicholson[1], Andrea Capa Salinas[2], Brenden R. Ortiz[2], Lawson Lloyd[3], Tommaso Pincelli[3], Tulio de Castro[1], Martin Wolf[1], Ralph Ernstorfer[3], Stephen D. Wilson[2], and Laurenz Rettig[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Materials Department and California Nanosystems Institute, University of California Santa Barbara, Santa Barbara, California 93106, USA — [3]Institut für Optik und Atomare Physik, Technische Universität Berlin, 10623 Berlin, Germany

The Kagome metal family AV3Sb5 (A=K, Rb, Cs) features an unconventional superconducting phase, coexisting with a parent charge density wave (CDW) phase. The origin of the CDW is still under debate. Moreover, this family exhibits a number of Van Hove Singularities (VHS) and a flat-band (FB) below the Fermi level, offering a unique platform for high electronic correlation. In order to gain insight into these properties, we study the ultrafast dynamics in CsV3Sb by using time and angle-resolved photoemission spectroscopy (trARPES). We discuss the ultrafast melting of CDW order, concomitant with a shift and a broadening for both the FB and the VHS, all being modulated by coherent phonon modes.

O 99.4 Fri 11:15 H11

**Ultrafast Nonequilibrium Dynamics of Room Temperature Charge Density Wave Fluctuations in 1T-$TiSe_2$** — •Hibiki Orio[1], Samuel Beaulieu[2], Sarath Sasi[2], Akib Jabed[2], Muthu P.T. Masilamani[1], Maximilian Ünzelmann[1], Jan Minar[3], Friedrich Reinert[1], Kai Rossnagel[4], Sotirios Fragkos[2], and Jakub Schusser[1,3] — [1]Universität Würzburg, Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence, Würzburg, Germany — [2]Université de Bordeaux - CNRS - CEA, CELIA, Talence, France — [3]New Technologies-Research Center, University of West Bohemia, Pilsen, Czech Republic — [4]Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany

$TiSe_2$ exhibits a 2×2×2 charge density wave (CDW) phase below 200 K, driven by the interplay between electron-hole and electron-lattice interactions. Nanoscale CDW domains, referred to as CDW fluctuations, persist even above the transition temperature. This exotic phase provides an intriguing platform for exploring the robustness of electron-hole interactions and electron-phonon coupling at elevated temperatures. Using time- and polarization-resolved XUV momentum microscopy, we investigate CDW fluctuations in $TiSe_2$ and their ultrafast light-induced dynamics. Our band structure mapping reveals that the backfolded Se 4p band associated with the CDW phase remains detectable even at room temperature. Furthermore, we demonstrate the ultrafast melting of these CDW fluctuations on an electronic timescale, followed by rapid recovery modulated by coherent amplitude phonon modes.

O 99.5 Fri 11:30 H11

**Coherent phonons and quasiparticle renormalization in semimetals from first principles** — •Christoph Emeis, Stephan Jauernik, Sunil Dahiya, Yiming Pan, Carl E. Jensen, Petra Hein, Michael Bauer, and Fabio Caruso — Kiel University, Germany

Coherent phonons offer a powerful means to manipulate structural and electronic properties of materials on ultrafast timescales, making them a key tool for exploring light-induced phase transitions and non-equilibrium dynamical phenomena.

We present an *ab initio* theory for the displacive excitation of coherent phonons in semimetals. We formulate a computational workflow for modelling light-induced structural changes and the resulting transient band-structure renormalization following excitation with a femtosecond laser. This framework is based on first-principles simulations of ultrafast electron and coherent phonon dynamics in the presence of electron-phonon interactions. We validate our approach through a combined theoretical and experimental study of coherent phonons in the semimetal antimony. The robust agreement between photoemission experiments and simulations corroborates our approach and paves the way for new opportunities to control structural and electronic degrees of freedom in semimetals via coherent phonon excitation.

C. Emeis *et al.* arXiv:2407.17118

O 99.6 Fri 11:45 H11

**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[1,3], Uwe Bovensiepen[1,3], and Michael Horn-von Hoegen[1,3] — [1]Department of Physics, University of Duisburg-Essen, Germany — [2]Department of Physical Chemistry, Fritz Haber Institute, Germany — [3]Center for Nanointegration Duisburg-Essen, Germany

In condensed matter, microscopic excitations interact on ultrafast time scales. The combination of suitable time domain experiments allows the analysis of processes such as the energy transfer from electrons to the nuclei subsequent to femtosecond laser pulse excitation. In this study, we used 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). While the electrons lose their excess energy within 400 fs, the lattice vibrational displacements gradually increase over 3-8 ps. Within the time gap, the energy is transiently stored in high-frequency phonon modes as simulated in a three-temperature model. Their temperature is experimentally accessible by the transient electron temperature after equilibration with such hot phonons. The excitation of low-frequency phonons and the subsequent thermalization and equilibration of the lattice are facilitated by anharmonic phonon-phonon coupling within the Pb film.

O 99.7 Fri 12:00 H11

**Resolving ultrafast atomic motion in WTe$_2$** — •Hanqian Lu[1,2], Victoria C. A. Taylor[2], Hyein Jung[1,2], Jannik Malter[1,2], Ralph Ernstorfer[1,2], and Yoav W. Windsor[1,2] — [1]Technische Universität Berlin, 10623 Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, 14195 Berlin, Germany

WTe$_2$ is a layered transition metal dichalcogenide with a distorted layered structure leading to distinct material properties. Here we study its lattice dynamics following ultrafast photoexcitation, using femtosecond electron diffraction (FED). We observe a strong coherent lattice response as well as growth of incoherent atomic vibrations, which we qualitatively describe as previously done. With the goal of describing such motions microscopically, we develop a quantitative model that extracts both the coherent and the incoherent atomic motions of each W and Te atom in the unit cell.

O 99.8 Fri 12:15 H11

**Structural dynamics of the silicon (111)-(7×7) surface upon optical excitation studied by ultrafast reflection high-energy electron diffraction** — •Jonas Darius Fortmann[1], Birk Finke[1], Christian Brand[1], and Michael Horn-von Hoegen[1,2] — [1]Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg

We present first results on the ultrafast structural dynamics of the Si(111)-(7×7) surface subsequent to an optical excitation. The surface is excited by an 800 nm fs-laser pulse at various fluences. The structural dynamics is followed through ultrafast reflection high-energy electron diffraction (URHEED) at a sample temperature of 80 K by means of the Debye-Waller effect. The surface has been excited for incident fluences $> 1.6\,\mathrm{mJ/cm^2}$ at a drop of RHEED intensity by only 0.8%. For the highest fluence of $5.4\,\mathrm{mJ/cm^2}$ the intensity drop was 2% which is equivalent to a rise of surface temperature by 7 K. The fluence dependence is explained by linear absorption through the metallic surface state of the 7×7 reconstruction. For higher fluences we observe an additional three photon absorption due to bulk excitation in order to overcome the direct bandgap. The recovery to the groundstate occur via several processes at different time constants. The system has not fully recovered the groundstate after $200\,\mu$s, which indicates the population of a long-lived electronic state.

O 99.9 Fri 12:30 H11

**Ultrafast imaging ellipsometry or interferometry - Which one is more suitable to measure the dielectric function of laser-excited materials?** — •Markus Olbrich, Theo Pflug, Andy Engel, and Alexander Horn — Laserinstitut Hochschule Mittweida, Hochschule Mittweida, Technikumplatz 17, 09648 Mittweida, Germany

Changes of the dielectric function of materials due to excitation by ultrafast laser radiation are crucial for understanding fundamental processes such as absorption of electromagnetic radiation or the relaxation of the excited electrons resulting in changes in the density of state of the material. The transient dielectric function can either be measured by ultrafast ellipsometry or interferometry. This study evaluates the advantages and disadvantages of each method exemplarily for an excited thin gold film induced by ultrafast laser radiation ($\lambda = 800\,\mathrm{nm}$, $\tau_H = 40\,\mathrm{fs}$) at fluences below and above the ablation threshold. The focus of the presentation is on characterizing the methodology including the experimental effort, the obtained signal-to-noise ratio, the data evaluation particularly in the limits of the applied optical model, as well as the physical interpretation of the measured data.

O 99.10 Fri 12:45 H11

**Anisotropic electronic response in hexagonal boron nitride to laser excitations from real-time time-dependent density functional theory** — •Cheng Wang, Markus E. Gruner, and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

Hexagonal boron nitride (h-BN) has a graphite-derived structure where nitrogen (N) and boron (B) atoms occupy alternating sites. In the framework of real-time time-dependent density functional theory (RT-TDDFT), as implemented in the Elk code, we systematically study the response of bulk and single layer h-BN to laser pulses with in- and out-of-plane polarization, different photon energies, duration and fluences. Our analysis focuses on transient charge redistribution and changes in occupation numbers, revealing a marked dependence on both polarization and frequency in bulk and monolayer h-BN. For a photon energy of 4.8 eV, slightly above the DFT band gap, we find a notable charge transfer from N to B $p_z$-orbitals in both bulk and monolayer for in-plane polarization. At 9.5 eV, excitations occur primarily between occupied and unoccupied N $p_x$-orbitals with a small charge transfer to B. In the monolayer, these excitations are suppressed for out-of-plane polarization. Finally, we compare our findings for monolayer h-BN with analogous calculations for graphene.

We gratefully acknowledge the funding provided by the DFG through CRC 1242, project C02. We acknowledge computation time at the MagnitUDE and AmplitUDE HPC systems at the University of Duisburg-Essen.

## O 100: Focus Session Chemical Imaging for the Elucidation of Molecular Structure II (joint session O/BP)

Unravelling the multiscale molecular heterogeneity at interfaces is one of the main challenges in modern biophysics and surface science due to the major role specific structural properties play in determining their macroscopic function and behavior. In the last few decades, several specialized chemical imaging techniques have been developed that can reveal many of these crucial structural details, representing an enormous advance in our elucidative capabilities. Clear examples of this range from super-resolution and 3D tomography to tag-free characterization down to the single-molecule level. This focus session will explore the vast range of methods and possibilities for characterizing the different structural aspects in heterogeneous molecular systems and specifically highlight the potential complementarity of the different techniques through multi-modal approaches. Overall, by bringing together different communities, this session aims to foster scientific exchanges that could spark the next major developments in chemical imaging.

Organized by
Martin Thämer (FHI Berlin), Alexander Fellows (FHI Berlin), and Kerstin Blank (University Linz)

Time: Friday 10:30–12:45 Location: H24

**Invited Talk** O 100.1 Fri 10:30 H24

**Multidimensional Super-resolution Imaging: Wasting Light to Learn New Things** — •Steven Lee — University of Cambridge

The talk will outline two single-molecule fluorescence approaches that can be used to determine orthogonal metrics about a single emitter.

The first half introduces ”POLCAM,” a simplified single-molecule orientation localization microscopy (SMOLM) method based on polarised detection using a polarisation camera. POLCAM’s fast algorithm operates over 1000 times faster than the current state-of-the-art, allowing near-instant determination of molecular anisotropy. To aid adoption, open-source image analysis software and visualization tools were developed. POLCAM's potential was demonstrated in studying alpha-synuclein fibrils and the actin cytoskeleton of mammalian cells. (Nature Methods 2024). The second approach focuses on "Single-Molecule Light Field Microscopy" (SMLFM), encoding 3D positions into 2D images for volumetric super-resolution microscopy. SMLFM shows an order-of-magnitude speed improvement over other 3D PSFs, resolving overlapping emitters through parallax. Experimental results reveal high accuracy and sensitivity in point detection, enabling whole-cell imaging of single membrane proteins in live primary B cells and high-density volumetric imaging in dense cytosolic tubulin datasets. (Nature Comms 2024)

**Invited Talk** O 100.2 Fri 11:00 H24

**MALDI mass spectrometry imaging: application examples ranging from food analysis to pharmaceutical research** — •Andreas Römpp — Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany

Mass spectrometry imaging is an analytical technique that provides spatially-resolved molecular information for a wide range of compound classes. In contrast to many histological methods, it does not require labeling. The capabilities and limitations of MS imaging will be discussed on the basis of several application areas with a focus on food analysis and pharmaceutical research. In our study 'MALDI mass spectrometry imaging: from constituents in fresh food to ingredients, contaminants and additives in processed food' (https://doi.org/10.1016/j.foodchem.2022.132529) we analyzed a range of plant-based and meat-based food. The analysis of natamycin in cheese and acrylamide in gingerbread constitute the first mass spectrometry imaging measurements of a food additive and a food contaminant, respectively. MS imaging is the only method that can analyze the distribution of drug compounds in animal models or human tissue (without labeling). This is exemplified on the detection of anti-tuberculosis drugs in mouse model tissue including our most recent study on the clinical stage antibiotic BTZ-043 which has just been accepted for publication in Nature Communications (https://doi.org/10.1038/s41467-025-56146-9).

O 100.3 Fri 11:30 H24

**On-Surface Synthesis and Characterization of a Nitrogen-Containing Heterocycle** — •Marco Thaler[1], Ricardo Ruvalcaba Briones[2], Matthias Zeilerbauer[1], Shadi Fatayer[2], and Laerte Patera[1] — [1]University of Innsbruck, Austria — [2]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Nitrogen-containing heterocycles are fundamental building blocks in nature, forming the core of essential biomolecules and pharmaceuticals. This study demonstrates the on-surface formation of an N-heterocyclic organic compound via thermal activation of a tailored precursor. High-resolution non-contact atomic force microscopy (nc-AFM) provides bond-level resolution of the synthesized structures. Complementary scanning tunneling spectroscopy visualizes changes in the electronic structure resulting from the formation of the heterocycle. Density functional theory calculations (DFT) reveal the most probable reaction mechanism, highlighting the critical role of hydrogen release as the driving force of the reaction. These findings emphasize the versatility of on-surface synthesis as a powerful tool for creating complex organic compounds.

O 100.4 Fri 11:45 H24

**Elasticity Mapping of Nonahelicene with Submolecular Resolution by NC-AFM** — •Max Halbauer[1], Takashi Kumagai[2], Martin Wolf[1], and Akitoshi Shiotari[1] — [1]Fritz-Haber-Institute, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institute for Molecular Science, 38 NishigoNaka, Myo-daiji, Okazaki 444-8585, Japan

Controlled modification of atomic configurations of molecules and materials is an exciting goal for non-contact atomic force microscopy (NC-AFM). Certain changes like shifts of the electronic energy gaps may be expected, but are not well explored and not established on the molecular scale. Here we report quantitative measurement of atomic-scale deformation in single molecules with NC-AFM. Individual molecules of nonahelicene ([9]H) and coronene (Cor) were studied on a Ag(110) surface under ultrahigh vacuum and cryogenic conditions by the measurement of frequency-shift distance curves for this. The molecular responses can be replicated with an empirical Lennard-Jones model, but for [9]H an elastic contribution is required to account for its elastic nature. Furthermore, a 3D-force mapping technique, termed molecular deformation mapping (MDM), allows to study the lateral position dependence of the elastic response. The MDM of [9]H reveals a spatially strongly anisotropic behaviour for the elasticity, interaction forces, elongation and binding energy of the tip to the molecule. The result is rationalized in terms of an aromaticity model.

O 100.5 Fri 12:00 H24

**Detection and control of quantum proton ordering in hydrogen bonds at the atomic scale** — •Yiqi Zhang — Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Directly probing the spatial arrangements and quantum nature of protons in hydrogen-bonded (H-bonded) materials and biosystems is the key to understand their macroscopic properties and functions. Here, exploiting bond-resolved atomic force spectroscopy (BR-AFS) combined with path-integral molecular dynamics method, we demonstrate for the first time that BR-AFS measurements along the apparent H-bond between proton donor and acceptor atoms allows the identification of both classical H-bonds with inherent directionality and non-classical H-bonds with quantum proton delocalization in self-assembled imidazole derivatives on surfaces. Unlike the conventional unidirectional H-bonding in linear chains, chiral cyclic hexamers exhibit unique quantum proton ordering in their ground states, which contain a mix of classical and non-classical H-bonds, breaking rotational symmetry. Furthermore, we show the capability to switch the quantum-proton-ordering state on and off by altering the adsorption registry coupled with a collective transfer of six protons within the cyclic H-bonds. These findings open new pathways for detecting and controlling complex proton orders and for engineering proton-based quantum states with atomic-level precision.

O 100.6 Fri 12:15 H24

**Imaging of the conformations of individual $\beta$-cyclodextrins with non-contact AFM** — Marko Grabarics[1], •Benjamin Mallada[1,2,3], Shayan Edalatmanesh[2,3], Stephan Rauschenbach[1], Pavel Jelinek[2,3], and Bruno de la Torre[2] — [1]Kavli Institute for Nanoscience Discovery, University of Oxford, UK — [2]CATRIN, Palacký University Olomouc, CZ — [3]Institute of Physics, Czech Academy of Sciences, CZ

Glycans, biopolymers essential to biology and materials science, are highly complex due to their structural diversity, conformational flexibility, and numerous possible isomers. Conventional methods often struggle to resolve these structures with atomic precision, especially under solvent-free conditions. We employ nc-AFM under UHV to determine the atomic structure of $\beta$-cyclodextrin ($\beta$-CD), a cyclic glucose molecule.

Our results reveal the adsorption geometries, hydroxy group positions, and stabilizing hydrogen bonds on a Au(111) surface. The primary face forms a closed hydrogen-bond network, while the secondary face exhibits pairwise interactions between OH groups of the same glucose monomer. DFT calculations validate these findings, enabling precise structural assignment and capturing subtle conformational differences.

This work highlights nc-AFM's capability to overcome the limitations of conventional sequencing techniques and represents the first application of nc-AFM to glycans. Future integration with ion deposition techniques could extend its utility to more complex glycans.

O 100.7 Fri 12:30 H24

**Domain size effects in the spectra of micro-heterogeneous samples** — •Thomas Mayerhöfer[1,2] and Jürgen Popp[1,2] — [1]Leibniz Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, 07745 Jena, Germany — [2]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University, Helmholtzweg 4, 07743 Jena, Germany

Samples are often not composed of a single pure compound but are instead mixtures of different substances. Under the Bouguer-Beer-Lambert approximation, the absorbance spectra of such mixtures can be simply derived by summing the spectra of the individual components, with each spectrum weighted by the molar fraction of the corresponding compound.

In the context of wave optics, the resolving power of light at a given wavelength becomes crucial. If a microscope using light at this wavelength can distinguish structural details within the sample, the sample is classified as micro-heterogeneous. In this case, spatial averaging occurs at the intensity level, involving reflectance and transmittance rather than absorbance.

The shift from micro-heterogeneity to macro-heterogeneity is gradual and cannot be described by an analytical formula due to the wave nature of light. This has significant implications for spectrum interpretation, as it can lead to substantial variations in peak shapes, positions, and intensities, e.g., during mitosis.

## O 101: Topology and Symmetry-protected Materials (joint session O/TT)

Time: Friday 10:30–12:15 Location: H25

O 101.1 Fri 10:30 H25

**Topological material in the III–V family: heteroepitaxial InBi on InAs** — •L. Nicolaï[1], J. Minár[1], M.C. Richter[2,3], O. Heckmann[2,3], J.-M. Mariot[4], U. Djukic[2], J. Adell[5], M. Leandersson[5], J. Sadowski[6], J. Braun[7], H. Ebert[7], J.D. Denlinger[8], I. Vobornik[9], J. Fujii[9], P. Šutta[1], G.R. Bell[10], M. Gmitra[11,12], and K. Hricovini[2,3] — [1]Univiversity of West Bohemia — [2]CY Cergy-Paris Université — [3]Université Paris-Saclay — [4]Sorbonne Université — [5]Lund University — [6]Polish Academy of Sciences — [7]LMU München — [8]ALS — [9]Istituto Officina dei Materiali, CNR — [10]University of Warwick — [11]Pavol Jozef Šafárik University in Košice — [12]Slovak Academy of Sciences

InBi(001) is formed epitaxially on InAs(111)-A by depositing Bi on to an In-rich surface. ARPES measurements reveal topological electronic surface states, close to the $\overline{\text{M}}$ high symmetry point. InBi surprisingly shows coexistence of Bi and In surface terminations. For the Bi termination, the study gives a consistent physical picture of the topological surface electronic structure of InBi(001) terminated by a Bi bilayer rather than a surface formed by splitting to a Bi monolayer termination. Theoretical calculations based on relativistic DFT and the one-step model of photoemission clarify the relationship between the InBi(001) surface termination and the topological surface states, supporting a predominant role of the Bi bilayer termination. Furthermore, a tight-binding model based on this Bi bilayer termination with only Bi–Bi hopping terms gives a deeper insight into the spin texture[1]. [1] Nicolaï *et al.* Phys. Rev. Research 6.4 (2024): 043116.

O 101.2 Fri 10:45 H25

**Hidden spin-texture in an inversion-symmetric Dirac crystal** — Kenta Hagiwara[1,2], Peter C. Schmitz[1], Philipp Rüssmann[1], Xin Liang Tan[1,2], Ying-Jiun Chen[3], Kui-Hon Ou Yang[4], Raman Sankar[5], Chien Jing[4], Yi-Hsin Shen[4], Mahmoud Zeer[1], Dongwook Go[6], Iulia Cojocariu[1], Daniel Baranowski[1], Vitaliy Feyer[1], Minn-Tsong Lin[1,6], Stefan Blügel[1], Claus M. Schneider[1,2], Yuriy Mokrousov[1,5], and •Christian Tusche[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, — [2]Faculty of Physics, University of Duisburg-Essen — [3]Ernst Ruska-Centre, Forschungszentrum Jülich — [4]Department of Physics, National Taiwan University, Taipei, Taiwan — [5]Academia Sinica, Taipei, Taiwan — [6]Johannes-Gutenberg University Mainz

A hidden spin polarization refers to a local spin polarization caused by apparent symmetry breaking and offers new perspectives for spintronics applications. Transition metal dichalcogenides can host various topological phases depending on the symmetry of their crystal structure. Here, by means of spin-resolving momentum microscopy, we reveal the spin texture of both topologically and symmetrically distinct surface and bulk Dirac cones in the inversion symmetric Dirac semimetal $\text{NiTe}_2$. We discovered a "hidden" spin polarization the bulk Dirac cone, localized at the different Te layers of the inversion symmetric bulk unit cell, such that the overlap of the two states results in a topologically trivial Dirac cone enforced by the global crystal symmetry. This work establishes a link between topology, spin-texture, and symmetry, enabling control by external perturbations.

O 101.3 Fri 11:00 H25

**Edge spectroscopy of the quantum spin Hall insulator indenene** — •Jonas Erhardt[1,2], Mattia Ianetti[3], Gianni Profeta[3], Domenico Di Sante[4], 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 — [3]Department of Physical and Chemical Sciences, University of L'Aquila — [4]Department of Physics and Astronomy, University of Bologna — [5]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

The non-trivial topology of the quantum spin Hall insulator indenene was recently demonstrated through bulk probes that reveal its topological band ordering [1,2]. According to the bulk-boundary correspondence, this ensures the existence of robust metallic states confined to the edge of this triangular indium monolayer. In this study, we employ scanning tunneling spectroscopy to investigate all three edge types of indenene for this correspondence. Our results demonstrate metallic edge density of states with suppressed backscattering near the bulk band gap, providing strong evidence for the existence of topologically protected edge states in indenene.

[1] M. Bauernfeind, J. Erhardt, and P. Eck *et al.*, Nat. Commun. **12**, 5396 (2021)

[2] J. Erhardt *et al.*, Phys. Rev. Lett. **132**, 196401 (2024)

O 101.4 Fri 11:15 H25

**Bismuthene at the Graphene/SiC Interface: A Protected Quantum Spin Hall Insulator** — •Niclas Tilgner[1], Susanne Wolff[1], Serguei Soubatch[2], Andres D. P. Unigarro[1], Sibylle Gemming[1], F. Stefan Tautz[2], Christian Kumpf[2], Thomas Seyller[1], Fabian Göhler[1], and Philip Schädlich[1] — [1]Institute of Physics, Chemnitz University of Technology, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany

Quantum spin Hall insulators (QSHIs) hold the potential to revolutionize next-generation technologies. Kane and Mele identified 2D honeycomb structures of heavy atoms with strong spin-orbit coupling as promising candidates for these materials. To realize this potential, however, the QSHI must be shielded from environmental influences. Previous research has demonstrated the intercalation of 2D Bi layers beneath graphene on SiC, resulting in the formation of two distinct phases. Among those, the $\beta$-phase exhibits a $(\sqrt{3} \times \sqrt{3})R30^\circ$ periodicity relative to the substrate. We identify the Bi adsorption site using x-ray standing wave imaging, a method which deterimes the element specific, 3D atomic distribution with respect to the bulk unit cell. After subsequent hydrogen intercalation, the Bi position changes significantly from hollow to top site adsorption. Further measurements with angle-resolved photoelectron spectroscopy reveal the band structure of the QSHI bismuthene with a pronounced Rashba splitting and slight p-type doping. We propose that the initial $\beta$-phase has to be considered as an electronically inactive layer of bismuthene, whose electronic structure can be established by subsequent hydrogen intercalation.

O 101.5 Fri 11:30 H25

**Probing the Electronic Structure at the Boundary of Topological Insulators in the Bi2Se3 Family by Combined STM and AFM** — •Christoph S. Setescak[1], Irene Aguilera[2], Adrian Weindl[1], Matthias Kronseder[1], Andrea Donarini[1], and Franz J. Giessibl[1] — [1]University of Regensburg, Regensburg, Germany — [2]University of Amsterdam and European Theoretical Spectroscopy Facility (ETSF), Amsterdam, The Netherlands

We develop a numerical scheme for the calculation of tunneling current I and differential conductance dI/dV of metal and CO terminated STM tips on the topological insulators Bi2Se3, Bi2Te2Se and Bi2Te3 and find excellent agreement with experiment. The calculation is an application of Chen's derivative rule, whereby the Bloch functions are obtained from Wannier interpolated tightbinding Hamiltonians and maximally localized Wannier functions from first-principle DFT+GW calculations. We observe signatures of the topological boundary modes, their hybridization with bulk bands, Van Hove singularities of the bulk bands and characterize the orbital character of these electronic modes using the high spatial resolution of STM and AFM. Bare DFT calculations are insufficient to explain the experimental data, which are instead accurately reproduced by many-body corrected GW calculations.

O 101.6 Fri 11:45 H25

**Revealing higher-order topological bulk-boundary correspondence in Bi crystals with spin-helical hinge state loop and proximity superconductivity** — •Dongming Zhao[1], Yang Zhong[1], Tian Yuan[1], Haitao Wang[1], Tianxing Jiang[1], Yang

Qi[1], Hongjun Xiang[1,2,3], Xingao Gong[1,2,3], Donglai Feng[2,3,4], and Tong Zhang[1,2,3,4] — [1]Fudan University, Shanghai, China — [2]Collaborative Innovation Center for Advanced Microstructures, Nanjing, China — [3]Shanghai Research Center for Quantum Sciences, Shanghai, China — [4]Hefei National Laboratory, Hefei, China

Topological materials are typically characterized by gapless boundary states, known as bulk-boundary correspondence. Recently, this concept has been generalized in higher-order topological insulators (HOTIs). E.g., a 2nd-order 3D TI hosts 1D topological hinge states winding around the crystal. A complete verification of HOTI will require probing all crystal boundaries. Here we studied a promising candidate of 2nd-order TI, Bi, in the form of mesoscopic crystals grown on superconducting V3Si. Using low-temperature STM, we directly observed dispersive 1D states on various hinges. Upon introducing magnetic scatterers, new scattering channels emerged selectively on certain hinges, revealing their spin-helical nature. Combining first-principle calculation and global symmetry analysis, we find these hinge states topological and formed a closed loop encircling the crystal. This provides direct evidence on the HOTI in Bi. Moreover, proximity superconductivity is observed in the topological hinge states serving as a promising platform for realizing topological superconductivity.

O 101.7 Fri 12:00 H25

**Simultaneous Atomic-Scale Imaging and Electronic Characterization of Wet-Chemically Prepared $Bi_2Se_3$ Nanoplatelets**

— •Auke Vlasblom, Victor Wesselingh, Jara Vliem, Daniel Vanmaekelbergh, and Ingmar Swart — Utrecht University, Utrecht, The Netherlands

Colloidal semiconductor nanoparticles are of great interest for various optoelectronic applications, such as integration in displays, solar cells and electronics. For applications, the surface of nanoparticles is of critical importance. However, until now, no technique exists to simultaneously investigate the atomic structure (e.g. the presence of defects) and the electronic properties of a nanoparticle, foremost limited by the presence of ligands that prevent direct access to the surface with a local probe. Here, we present a new and widely applicable procedure that allows investigation of the surface of a nanoparticle with a local probe. Using this method, nanoparticles are transferred to an atomically clean substrate under ultra-high vacuum conditions. We demonstrate the procedure for topological two-dimensional $Bi_2Se_3$ nanoplatelets deposited on Au(111). We reveal the atomic and electronic structure of the surface of colloidally synthesised $Bi_2Se_3$ nanoplatelets with scanning tunneling microscopy and spectroscopy measurements. In this talk, I will highlight the various types of defects that occur at the (sub-)surface of $Bi_2Se_3$ nanoplatelets and I will show their influence on the electronic structure.

## O 102: Closing Talk Andreas Heinrich

Time: Friday 13:15–14:00 Location: H1

**Topical Talk** O 102.1 Fri 13:15 H1

**Quantum sensing with atomic-scale spatial resolution**

— •Andreas Heinrich — IBS Center for Quantum Nanoscience, Seoul, Korea

There is a strong international research effort in the area of quantum nanoscience, where the concepts of quantum coherence, superposition and entanglement of quantum states are exploited in solid state and molecular systems. One of the very prominent applications in this realm is Quantum Sensing, where a quantum system is used to measure some external fields with high energy and high spatial resolution. In this talk we will focus on quantum-coherent experiments in Scanning Tunneling Microscopy (STM). STM enables the study of surfaces with atomic-scale spatial resolution and offers the ability to study individual atoms and molecules on surfaces. To make a movable quantum sensor with atomic-scale spatial resolution, we attached a single molecule of PTCDA to the spin-polarized apex of an STM tip. In contrast to all other known molecules, its coupling to the tip is so weak that this molecule performs as an excellent electron spin resonance (ESR) sensor on a bare metallic surface. We show how this sensor can be used to measure atomic-scale magnetic and electric fields emanating from single atoms on a surface and compare its performance to the well-established NV center in diamond.

Taner Esat, Dmitriy Borodin, et al., A quantum sensor for atomic-scale electric and magnetic fields, Nature Nanotechnology (2024).

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