Surface Science Division
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

(Lecture halls CHE 89, CHE 91, GER 37, GER 38, GER 39, WIL A 213, REC C 213, TRE Phy, TRE Ma, HSZ 01 and HSZ 02; Poster P2/EG)

Plenary Talk

PLV V	Wed	8:30– 9:15	HSZ 01	**Advances in Ultrafast Electron Microscopy** — •Claus Ropers

Laureate of the Gaede Prize 2023

PRV II	Wed	13:15–13:45	HSZ 01	**Towards chemical and optical band structure engineering in molecular-based heterostructures** — •Benjamin Stadtmueller

Overview Talks

O 1.1	Mon	9:30–10:15	TRE Phy	**From surface structure to exciton evolution: a many-body theoretical perspective** — •Sivan Refaely-Abramson
O 27.1	Tue	9:30–10:15	TRE Phy	**Dive right in! Molecular insights into electrochemical surface science** — •Katrin F. Domke
O 44.1	Wed	9:30–10:15	TRE Phy	**Spins on Surfaces: A Gateway to the Quantum World** — •Christian R. Ast
O 71.1	Thu	9:30–10:15	TRE Phy	**Surface dynamics under reaction conditions** — •Edvin Lundgren
O 90.1	Fri	9:30–10:15	TRE Phy	**Molecular Surfaces With a Twist: Magnetochiral Asymmetries and Topological Self-Assembly** — •Karl-Heinz Ernst
O 98.1	Fri	13:15–14:00	HSZ 03	**Surfaces go topological – third generation 2D quantum materials** — •Ralph Claessen

Invited Talks of the joint Symposium Ultrafast Excitation Pathways of Quantum Materials (SYUE)

See SYUE for the full program of the symposium.

SYUE 1.1	Wed	9:30–10:00	HSZ 01	**Dynamics and control in quantum materials using multi-terahertz spectroscopy** — •Richard Averitt
SYUE 1.2	Wed	10:00–10:30	HSZ 01	**Accessing the nonthermal phonon populations in 2D materials with femtosecond electron diffuse scattering** — •Hélène Seiler, Marios Zacharias, Daniela Zahn, Patrick-Nigel Hildebrandt, Thomas Vasileiadis, Yoav William Windsor, Yingpeng Qi, Christian Carbogno, Claudia Draxl, Ralph Ernstorfer, Fabio Caruso
SYUE 1.3	Wed	10:30–11:00	HSZ 01	**Exciting potentials – Exploring the realms of ultrafast phase transitions** — •Laurenz Rettig
SYUE 1.4	Wed	11:15–11:45	HSZ 01	**Sub-cycle multidimensional spectroscopy of strongly correlated materials** — Viktor Valmispild, Evgeny Gorelov, Martin Eckstein, Alexander Lichtenstein, Hideo Aoki, Mikhail Katsnelson, Misha Ivanov, •Olga Smirnova

SYUE 1.5	Wed	11:45–12:15	HSZ 01	**Witnessing many-body entanglement in light-driven quantum materials** — •Matteo Mitrano, Denitsa Baykusheva, Mona Kalthoff, Damian Hofmann, Martin Claassen, Dante Kennes, Michael Sentef
SYUE 1.6	Wed	12:15–12:45	HSZ 01	**Optical responses of photoexcited materials: from parametric amplification to photoinduced superconductivity** — •Eugene Demler

Invited Talks of the joint Symposium Physics of van der Waals 2D Heterostructures (SYHS)

See SYHS for the full program of the symposium.

SYHS 1.1	Fri	9:30–10:00	HSZ 01	**Novel moiré excitons and ultrafast optical dynamics in van der Waals 2D heterostructures** — •Steven G. Louie
SYHS 1.2	Fri	10:00–10:30	HSZ 01	**Interaction induced magnetism in 2D semiconductor moiré superlattices** — •Xiaodong Xu
SYHS 1.3	Fri	10:30–11:00	HSZ 01	**Ions in tight places: intercalation and transport of ions in van der Waals heterostructures** — •Irina Grigorieva
SYHS 1.4	Fri	11:15–11:45	HSZ 01	**Spin-orbit proximity in van der Waals heterostructures** — •Felix Casanova
SYHS 1.5	Fri	11:45–12:15	HSZ 01	**Plethora of many-body ground states in magic angle twisted bilayer graphene** — •Dmitri Efetov

Topical Talks of the Focus Session "Frontiers of Electronic-Structure Theory" (joint Session O/HL)

O 9.3	Mon	11:00–11:30	TRE Ma	**Large-scale machine-learning assisted discovery and characterization of materials** — •Miguel Alexandre Lopes Marques
O 17.1	Mon	15:00–15:30	TRE Ma	**Coupled-cluster theory for complex solids made ready** — •Andreas Grüneis
O 35.4	Tue	11:15–11:45	TRE Ma	**Towards low-scaling GW calculations for 2D materials** — •Jan Wilhelm
O 53.2	Wed	10:45–11:15	TRE Ma	**TREX: an integrated HPC software platform for quantum Monte Carlo calculations** — •Claudia Filippi
O 61.5	Wed	16:15–16:45	TRE Ma	**Challenges in modelling correlated electronic matter** — •Roser Valenti
O 79.3	Thu	11:00–11:30	TRE Ma	**New Opportunities for First Principles Simulations of Thousands of Atoms Using Linear Scaling Density Functional Theory** — •Laura Ratcliff

Topical Talks of the Focus Session "Ion Beam Interaction with Surfaces and 2D Materials"

O 5.1	Mon	10:30–11:00	GER 38	**Highly charged, slow and swift ions interacting with surfaces and 2D materials** — •Marika Schleberger
O 5.4	Mon	11:30–12:00	GER 38	**A contactless single-step process for simultaneous nanoscale patterning and cleaning of large-area graphene** — •Tuan Tran
O 13.1	Mon	15:00–15:30	GER 38	**Space weathering of planetary surfaces** — •Peter Wurz
O 31.1	Tue	10:30–11:00	GER 38	**Ultra-low energy ion implantation of two-dimensional materials** — •Hans Hofsäss

Topical Talks of the Focus Session "Scanning Probe Microscopy with Quartz Sensors"

O 45.2	Wed	10:45–11:15	CHE 89	**Single-molecule reactions performed and characterized using atomic force microscopy** — •Leo Gross
O 54.1	Wed	15:00–15:30	CHE 89	**Peering into interfacial water by qPlus-based atomic force microscopy** — •Ying Jiang
O 54.5	Wed	16:15–16:45	CHE 89	**AFM with the qPlus sensor: An indeal tool for oxide surface science** — •Ulrike Diebold

O 87.1	Thu	15:00–15:30	TRE Ma	**Quartz-sensor detection for single-electron tunneling spectroscopy** — •Jascha Repp
O 87.5	Thu	16:15–16:45	TRE Ma	**Application of atomic force microscopy with quartz sensors to quantum states in graphene and related twisted heterostructures** — •Joseph Stroscio
O 97.4	Fri	11:15–11:45	TRE Ma	**Heteroatom-substituted and three-dimensional nanocarbon materials studied with low temperature STM and qPlus AFM** — •Shigeki Kawai

Topical Talks of the Focus Session "Semiconductor Surface Chemistry - from Reaction Mechanisms to Well-Ordered Interfaces"

O 48.1	Wed	10:30–11:00	GER 38	**Surface functionalization of semiconductors: Introducing spectroscopic labels, monolayer control for ultra-shallow doping, and providing surface passivation for atomically-precise processes** — •Andrew Teplyakov
O 48.3	Wed	11:15–11:45	GER 38	**Growth of organic monolayers on Si(111)** — •Martin Franz
O 57.1	Wed	15:00–15:30	GER 38	**Incorporation of arsenic into silicon (001) and germanium (001) for atomic-scale device fabrication.** — •Steven R. Schofield
O 57.3	Wed	15:45–16:15	GER 38	**Semiconductor surface chemistry towards hybrid interfaces with ab initio approaches** — •Ralf Tonner-Zech

Topical Talks of the Focus Session "Ultrafast Dynamics in Nanostructures"

O 75.1	Thu	10:30–11:00	GER 38	**Ultrafast nano-imaging: probing quantum dynamics in space and time** — •Markus Raschke
O 75.5	Thu	11:45–12:15	GER 38	**Lightwave-driven scanning tunneling microscopy and spectroscopy at the atomic scale** — •Vedran Jelic
O 83.1	Thu	15:00–15:30	GER 38	**Imaging ultrafast electron dynamics in isolated nanoparticles** — •Daniela Rupp
O 83.5	Thu	16:15–16:45	GER 38	**Ultrafast coherent manipulation of free electrons via quantum interaction with shaped optical fields** — •Giovanni Maria Vanacore

General Invited Topical Talks

O 7.1	Mon	10:30–11:00	REC C 213	**Superconductivity in atom-by-atom crafted quantum corrals** — •Lucas Schneider
O 10.1	Mon	15:00–15:30	CHE 89	**Photoemission Orbital Tomography: Imaging Molecular Wave Functions in Reciprocal and Real Space** — •F. S. Tautz
O 16.4	Mon	15:45–16:15	TRE Phy	**Microscopic insight into non-equilibrium dynamics through time-resolved x-ray absorption spectroscopy** — •Andrea Eschenlohr
O 33.1	Tue	10:30–11:00	REC C 213	**Fermi liquids, Luttinger integrals, topological invariants ... and magnetic molecules** — •Rok Zitko
O 34.6	Tue	11:45–12:15	TRE Phy	**Photoemission orbital tomography for excitons** — •Peter Puschnig
O 52.4	Wed	11:15–11:45	TRE Phy	**Modeling and Design of Single-Atom Alloy Catalysts** — •Mie Andersen
O 59.1	Wed	15:00–15:30	REC C 213	**Interplay of Inversion Symmetry Breaking and Spin-Orbit Coupling** — •Maximilian Ünzelmann
O 58.3	Wed	15:30–16:00	WIL A317	**Phase-locked photon-electron interaction without a laser** — •Nahid Talebi
O 55.6	Wed	16:15–16:45	CHE 91	**Towards Understanding and Controlling On-Surface Reactions and Self-Assembly Mechanisms** — •Daniel Ebeling
O 80.3	Thu	15:30–16:00	CHE 89	**Topological Plasmonics and Plasmonic Twistronics: Skyrmions, Merons, Quasicrystals, and Sykrmion Bags** — •Harald Giessen
O 86.3	Thu	15:30–16:00	TRE Phy	**Novel concepts to simulate electrified liquid/solid interfaces from first principles** — •Stefan Wippermann

Sessions

O 1.1–1.1	Mon	9:30–10:15	TRE Phy	**Overview Talk Sivan Refaely-Abramson**
O 2.1–2.10	Mon	10:30–13:00	CHE 89	**Organic Molecules on Inorganic Substrates I: Electronic, Optical and Other Properties I**
O 3.1–3.7	Mon	10:30–12:15	CHE 91	**Metal Substrates: Adsorption and Reaction of Small Molecules I**
O 4.1–4.8	Mon	10:30–12:30	GER 37	**Tribology: Surfaces and Nanostructures**
O 5.1–5.8	Mon	10:30–13:00	GER 38	**Focus Session: Ion Beam Interaction with Surfaces and 2D Materials I**
O 6.1–6.10	Mon	10:30–13:00	GER 39	**New Methods: Experiments and Theory**
O 7.1–7.9	Mon	10:30–13:00	REC C 213	**Spins on Surfaces at the Atomic Scale I**
O 8.1–8.9	Mon	10:30–12:45	TRE Phy	**Ultrafast Electron Dynamics at Surface and Interfaces I**
O 9.1–9.8	Mon	10:30–13:00	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory I (joint session O/HL)**
O 10.1–10.9	Mon	15:00–17:30	CHE 89	**Organic Molecules on Inorganic Substrates II: Electronic, Optical and Other Properties II**
O 11.1–11.9	Mon	15:00–17:15	CHE 91	**Surface Reactions**
O 12.1–12.8	Mon	15:00–17:00	GER 37	**Scanning Probe Techniques: Method Development I**
O 13.1–13.8	Mon	15:00–17:15	GER 38	**Focus Session: Ion Beam Interaction with Surfaces and 2D Materials II**
O 14.1–14.11	Mon	15:00–17:45	GER 39	**Nanostructures at Surfaces (joint session O/CPP)**
O 15.1–15.12	Mon	15:00–18:00	REC C 213	**Spins on Surfaces at the Atomic Scale II**
O 16.1–16.9	Mon	15:00–17:30	TRE Phy	**Ultrafast Electron Dynamics at Surface and Interfaces II**
O 17.1–17.7	Mon	15:00–17:15	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory II (joint session O/HL)**
O 18.1–18.9	Mon	18:00–20:00	P2/EG	**Poster: 2D Materials I**
O 19.1–19.9	Mon	18:00–20:00	P2/EG	**Poster: Ultrafast Electron Dynamics at Surface and Interfaces I**
O 20.1–20.11	Mon	18:00–20:00	P2/EG	**Poster: Spins and Magnetism at Surfaces**
O 21.1–21.7	Mon	18:00–20:00	P2/EG	**Poster: Scanning Probe Techniques**
O 22.1–22.9	Mon	18:00–20:00	P2/EG	**Poster Session: Organic Molecules on Inorganic Substrates I**
O 23.1–23.6	Mon	18:00–20:00	P2/EG	**Poster: Surface Reactions**
O 24.1–24.5	Mon	18:00–20:00	P2/EG	**Poster: Ion Beam Interaction with Surfaces and Interfaces**
O 25.1–25.5	Mon	18:00–20:00	P2/EG	**Poster: Metal Substrates**
O 26.1–26.8	Mon	18:00–20:00	P2/EG	**Poster: New Methods**
O 27.1–27.1	Tue	9:30–10:15	TRE Phy	**Overview Talk Katrin Domke**
O 28.1–28.10	Tue	10:30–13:00	CHE 89	**Organic Molecules on Inorganic Substrates III: Adsorption and Growth I**
O 29.1–29.10	Tue	10:30–13:00	CHE 91	**Supported Nanoclusters: Structure, Reactions and Catalysis**
O 30.1–30.11	Tue	10:30–13:15	GER 37	**2D Materials I: Electronic Structure**
O 31.1–31.8	Tue	10:30–12:45	GER 38	**Focus Session: Ion Beam Interaction with Surfaces and 2D Materials III**
O 32.1–32.9	Tue	10:30–12:45	GER 39	**Semiconductor Substrates**
O 33.1–33.9	Tue	10:30–13:00	REC C 213	**Spins on Surfaces at the Atomic Scale III**
O 34.1–34.10	Tue	10:30–13:15	TRE Phy	**Ultrafast Electron Dynamics at Surface and Interfaces III**
O 35.1–35.7	Tue	10:30–12:45	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory III (joint session O/HL)**
O 36.1–36.12	Tue	18:00–20:00	P2/EG	**Poster: 2D Materials II**
O 37.1–37.13	Tue	18:00–20:00	P2/EG	**Poster: Ultrafast Electron Dynamics at Surface and Interfaces II**
O 38.1–38.7	Tue	18:00–20:00	P2/EG	**Poster: Organic Molecules on Inorganic Substrates II**
O 39.1–39.6	Tue	18:00–20:00	P2/EG	**Poster Session: Heterogeneous Catalysis and Surface Dynamics**
O 40.1–40.4	Tue	18:00–20:00	P2/EG	**Poster: Semiconductor Substrates**
O 41.1–41.4	Tue	18:00–20:00	P2/EG	**Poster: Supported Nanoclusters**
O 42.1–42.12	Tue	18:00–20:00	P2/EG	**Poster: Nanostructures at Surfaces**
O 43.1–43.8	Tue	18:00–20:00	P2/EG	**Poster: Plasmonics and Nanooptics I**
O 44.1–44.1	Wed	9:30–10:15	TRE Phy	**Overview Talk Christian Ast**
O 45.1–45.7	Wed	10:30–12:30	CHE 89	**Focus Session: Scanning Probe Microscopy with Quartz Sensors I**
O 46.1–46.7	Wed	10:30–12:15	CHE 91	**Electron-Driven Processes at Surfaces and Interfaces**

O 47.1–47.10	Wed	10:30–13:00	GER 37	**2D Materials II: Growth, Structure and Substrate Interaction I**
O 48.1–48.5	Wed	10:30–12:15	GER 38	**Focus Session: Semiconductor Surface Chemistry – from Reaction Mechanisms to Well-Ordered Interfaces I**
O 49.1–49.9	Wed	10:30–12:45	WIL A317	**Plasmonics and Nanooptics I: Fabrication and Application**
O 50.1–50.4	Wed	10:30–11:30	REC C 213	**Spins on Surfaces at the Atomic Scale IV**
O 51.1–51.6	Wed	11:30–13:00	REC C 213	**Surface Magnetism**
O 52.1–52.8	Wed	10:30–12:45	TRE Phy	**Heterogeneous Catalysis and Surface Dynamics I**
O 53.1–53.8	Wed	10:30–13:00	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory IV (joint session O/HL)**
O 54.1–54.8	Wed	15:00–17:30	CHE 89	**Focus Session: Scanning Probe Microscopy with Quartz Sensors II**
O 55.1–55.10	Wed	15:00–17:45	CHE 91	**Organic Molecules on Inorganic Substrates IV: Adsorption and Growth II**
O 56.1–56.10	Wed	15:00–17:30	GER 37	**2D Materials III: Growth, Structure and Substrate Interaction II (joint session O/CPP)**
O 57.1–57.6	Wed	15:00–17:00	GER 38	**Focus Session: Semiconductor Surface Chemistry – from Reaction Mechanisms to Well-Ordered Interfaces II**
O 58.1–58.9	Wed	15:00–17:30	WIL A317	**Plasmonics and Nanooptics II: Light-Matter Interaction and Spectroscopy I**
O 59.1–59.10	Wed	15:00–17:45	REC C 213	**Electronic Structure of Surfaces I**
O 60.1–60.12	Wed	15:00–18:00	TRE Phy	**Solid-Liquid Interfaces I: Structure and Spectroscopy**
O 61.1–61.8	Wed	15:00–17:30	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory V (joint session O/HL)**
O 62.1–62.8	Wed	15:00–18:30	POT 81	**Focus Session: Wissenschaftskommunikation / Outreach (joint session HL/O/TT)**
O 63.1–63.2	Wed	18:00–20:00	P2/EG	**Poster: Data Management**
O 64.1–64.12	Wed	18:00–20:00	P2/EG	**Poster: Graphene**
O 65.1–65.6	Wed	18:00–20:00	P2/EG	**Poster: Topology and Symmetry-Protected Materials**
O 66.1–66.11	Wed	18:00–20:00	P2/EG	**Poster: Scanning Probe Microscopy with Quartz Sensors**
O 67.1–67.10	Wed	18:00–20:00	P2/EG	**Poster: Electronic Structure of Surfaces**
O 68.1–68.5	Wed	18:00–20:00	P2/EG	**Poster: Oxide and Insulator Surfaces**
O 69.1–69.14	Wed	18:00–20:00	P2/EG	**Poster: Solid-Liquid Interfaces**
O 70.1–70.10	Wed	18:00–20:00	P2/EG	**Poster: Plasmonics and Nanooptics II**
O 71.1–71.1	Thu	9:30–10:15	TRE Phy	**Overview Talk Edvin Lundgren**
O 72.1–72.5	Thu	10:30–13:00	CHE 89	**Gerhard Ertl Young Investigator Award Competition**
O 73.1–73.8	Thu	10:30–12:30	CHE 91	**Metal Substrates: Adsorption and Reaction of Small Molecules II**
O 74.1–74.9	Thu	10:30–12:45	GER 37	**2D Materials IV: Heterostructures (joint session O/CPP)**
O 75.1–75.9	Thu	10:30–13:15	GER 38	**Focus Session: Ultrafast Dynamics in Nanostructures I**
O 76.1–76.9	Thu	10:30–12:45	WIL A317	**Plasmonics and Nanooptics III: Light-Matter Interaction and Spectroscopy II**
O 77.1–77.9	Thu	10:30–12:45	REC C 213	**Scanning Probe Techniques: Method Development II**
O 78.1–78.9	Thu	10:30–12:45	TRE Phy	**Heterogeneous Catalysis and Surface Dynamics II**
O 79.1–79.7	Thu	10:30–12:45	TRE Ma	**Focus Session: Frontiers of Electronic-Structure Theory VI (joint session O/HL)**
O 80.1–80.8	Thu	15:00–17:15	CHE 89	**Plasmonics and Nanooptics IV: Light-Matter Interaction and Spectroscopy III**
O 81.1–81.12	Thu	15:00–18:00	CHE 91	**Oxide and Insulator Surfaces I: Adsorption and Reaction of Small Molecules**
O 82.1–82.9	Thu	15:00–17:15	GER 37	**Graphene I: Adsorption, Intercalation and Doping**
O 83.1–83.8	Thu	15:00–17:30	GER 38	**Focus Session: Ultrafast Dynamics in Nanostructures II**
O 84.1–84.11	Thu	15:00–18:30	WIL A317	**Focus Session: Making Experimental Data F.A.I.R. – New Concepts for Research Data Management I (joint session O/TT)**
O 85.1–85.11	Thu	15:00–17:45	REC C 213	**Electronic Structure of Surfaces II**
O 86.1–86.10	Thu	15:00–17:45	TRE Phy	**Solid-Liquid Interfaces II: Reactions and Electrochemistry I**
O 87.1–87.8	Thu	15:00–17:30	TRE Ma	**Focus Session: Scanning Probe Microscopy with Quartz Sensors III**
O 88	Thu	19:00–19:30	HSZ 01	**Members' Assembly**
O 89	Thu	19:30–20:30	HSZ 01	**Post-Deadline Session**

O 90.1–90.1	Fri	9:30–10:15	TRE Phy	**Overview Talk Karl-Heinz Ernst**
O 91.1–91.9	Fri	10:30–12:45	CHE 89	**Plasmonics and Nanooptics V: Waveguides and Antennas**
O 92.1–92.10	Fri	10:30–13:00	CHE 91	**Oxide and Insulator Surfaces II: Structure, Epitaxy and Growth**
O 93.1–93.8	Fri	10:30–12:30	GER 37	**Graphene II: Electronic Structure and Growth**
O 94.1–94.10	Fri	10:30–13:00	GER 38	**Topology and Symmetry-Protected Materials**
O 95.1–95.11	Fri	9:30–12:45	WIL A317	**Focus Session: Making Experimental Data F.A.I.R. – New Concepts for Research Data Management II (joint session O/TT)**
O 96.1–96.10	Fri	10:30–13:00	TRE Phy	**Solid-Liquid Interfaces III: Reactions and Electrochemistry II**
O 97.1–97.8	Fri	10:30–12:45	TRE Ma	**Focus Session: Scanning Probe Microscopy with Quartz Sensors IV**
O 98.1–98.1	Fri	13:15–14:00	HSZ 03	**Overview Talk Ralph Claessen**

Members' Assembly of the Surface Science Division

Thursday 19:00–19:30 HSZ 01

- Report of the Chairman
- Presentation of the Gerhard Ertl Young Investigator Award
- Miscellaneous

O 1: Overview Talk Sivan Refaely-Abramson

Time: Monday 9:30–10:15 Location: TRE Phy

Invited Talk O 1.1 Mon 9:30 TRE Phy

From surface structure to exciton evolution: a many-body theoretical perspective — •Sivan Refaely-Abramson — Weizmann Institute of Science, Rehovot, Israel

Excited-state processes involving Coulomb-bound electron-hole pairs in functional materials are essential for emerging applications, from energy conversion to quantum information science. The associated exciton creation and relaxation mechanisms are often coupled to optical selection rules, stemming from the underlying material structure. In this talk, I will discuss the relation between exciton evolution and structural modifications in monolayer semiconductors. Two broadly explored examples of such modifications are the introduction of atomic defects and the composition of layered heterostructures. Both offer controllable design pathways to induce long-lived, low-lying excitons with tunable spatial localization and spin polarization. These structure-sensitive exciton properties can be detected in a variety of experimental scenarios from absorption and luminescence under electric and magnetic fields to angle-resolved photoemission spectroscopy, allowing for a close inspection of the microscopic interaction mechanisms. I will present an overview of a many-body ab initio theoretical approach to capture and predict the involved excitonic phenomena and discuss our recent theory-experiment collaborations to explore these effects and their tunability through defect engineering and interlayer twisting.

O 2: Organic Molecules on Inorganic Substrates I: Electronic, Optical and Other Properties I

Time: Monday 10:30–13:00 Location: CHE 89

O 2.1 Mon 10:30 CHE 89

Hooke's law in a molecular spring: An nc-AFM and STM study of nonahelicene on Ag(110) — •Max Halbauer[1], Takashi Kumagai[2], Martin Wolf[1], and Akitoshi Shiotari[1] — [1]Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institute for Molecular Science, 38 Nishigo-Naka, Myodaiji, 444-8585 Okazaki, Japan

Helicenes are a class of conjugated aromatic molecules representing macroscopic springs on the molecular scale. However, experimental insights on their mechanical properties remain scarce. This contribution employs scanning tunneling microscopy (STM) and noncontact atomic force microscopy (nc-AFM) measurements (UHV, liq. He) in order to address this issue. Frequency shift-distance traces were acquired on individual nonahelicene molecules and a planar reference molecule (coronene) and converted subsequently to force-distance curves. Model-functions accounting for the elasticity of the molecule were fitted to the data, which yielded the spring-constant - k - for elongation of nonahelicene. This work shows therefore that Hooke's law can be verified on the single-molecule scale by nc-AFM.

O 2.2 Mon 10:45 CHE 89

Complex rotational behavior of ground and excited molecular states — •Andreas Christ, Markus Leisegang, Patrick Härtl, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The high sensitivity of molecular rotors to the intricate molecule–substrate interaction leads to a large variety of their rotational behavior [1]. In some cases this interaction can even change for different rotational positions on a molecule's rotation path. We have studied these dependencies for copper-phthalocyanine (CuPc) on Cu(111) by means of low-temperature scanning tunneling microscopy. In agreement with previous results [2,3], we find one ground state oriented along the high-symmetry axes of the substrate and two excited states tilted by ≈ ±7°. A more detailed analysis reveals an exceptionally low threshold of ≈ 20 meV for rotations between these three stable states. Interestingly, the interaction of the molecule with the substrate and therefore the rotation rate varies significantly between the ground and the excited states due to their different molecular bending. Additionally, we find two adsorption positions, which slightly lift the degeneracy between the two excited states.

[1] D. Lensen *et al.*, Soft Matter **8,** 9053 (2012)
[2] J. Schaffert *et al.*, Phys. Rev. B **88**, 075410 (2013)
[3] S. Fremy-Koch *et al.*, Phys. Rev. B **100**, 155427 (2019)

O 2.3 Mon 11:00 CHE 89

Current Driven Unidirectional Rotation of Geländer Molecule — •Štěpán Marek[1], Jan Wilhelm[2], Richard Korytár[1], and Ferdinand Evers[2] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Czech Republic — [2]Condensed Matter Theory Group, Institute of Physics, Faculty of Theoretical Physics, University of Regensburg, Bavaria, Germany

Rotations of molecules driven by current are possible basis for construction of molecular motors. In "Geländer" molecules, the chiral structure was thought to drive the momentum transfer from travelling electrons to the molecule. We construct a simple model, motivated by our DFT based study, to explore the structure of the current density in such a molecule and identify the regions of the molecule that contribute majority of the angular momentum of the electron current. We also discuss the particularities of our results, especially the conservation of rotation direction under the exchange of electric bias direction. The results are compared with experimental observations.

O 2.4 Mon 11:15 CHE 89

SPM Tip-induced Cleavage of Bridging Groups to Generate Carbon Nanomaterials — •Zilin Ruan[1], Tim Naumann[1], John B. Bauer[2], Lukas Heuplick[1], Holger F. Bettinger[2], and J. Michael Gottfried[1] — [1]Department of Chemistry, Philipps University Marburg, Hans-Meerwein-Straße 4, 35037 Marburg (Germany) — [2]Institut für Organische Chemie, Auf der Morgenstelle 18, 72076 Tübingen(Germany)

The on-surface synthesis of carbon nanomaterials is usually carried out on a metal surface by thermal activation, wherein the reaction selectivity and outcome are influenced by various factors. By contrast, manipulations with a scanning probe microscope (SPM) avoid these obstacles by electrically triggering the chemical transformation of individual molecules via the SPM tip due to electronic excitation or inelastic energy transfer. Here, using tip manipulation, we explore the suitability of the removal of etheno- and diastereomeric 1,2-diol moieties to generate acenes. Compared to other previously used leaving groups such as monoketone, diketone and oxo bridges, the here used bridges have certain advantages in the precursor synthesis, but are more challenging regarding their on-surface removal. Investigation of the various main and side reactions offer a deeper understanding of complex elimination and rearrangement reactions induced by SPM manipulation.

O 2.5 Mon 11:30 CHE 89

Illuminating an individual non-fluorescent molecule — •Tzu-Chao Hung[1,2], Yokari Godinez Loyola[3], Manuel Steinbrecher[1], Brian Kiraly[1], Alexander A. Khajetoorians[1], Nikos L. Doltsinis[3], Cristian A. Strassert[3], and Daniel Wegner[1] — [1]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands — [2]Department of Physics, University of Regensburg, Regensburg, 93040, Germany — [3]Physikalisches Institut and Center for Nanotechnology (CeNTech), Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Combining scanning tunneling microscopy, spectroscopy and STM-induced luminescence (STML) allows us to study the optoelectronic properties down to the atomic scale. Generalizing the atomic control and imaging capabilities of STML to phosphorescent or even non-fluorescent molecules can provide a new route to fundamentally understand the photophysical properties of an individual molecule. Nickel phthalocyanine (NiPc) is a non-fluorescent molecule. Light emission from the ligand-centered excited state known as Q-band is quenched due to fast relaxation into the nonradiative metal-centered excited state. Hence, the transition energy of the Q-band can only be determined by absorption spectroscopy. Here, we propose an alternative approach to activate radiative decay of the Q-band of NiPc by utilizing STML in combination with control of the local environment and discuss the involved excitation and relaxation pathways. We compare our results with optical spectroscopy and ab initio calculations and discuss the involved excitation and relaxation pathways.

O 2.6 Mon 11:45 CHE 89

STM-induced luminescence from single graphene nanoribbons — •Song Jiang[1], Tomáš Neuman[1,2], Alex Boeglin[1], Fabrice Scheurer[1], and Guillaume Schull[1] — [1]Université de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000 Strasbourg, France — [2]Institut des Sciences Moléculaires d'Orsay (ISMO), UMR 8214, CNRS, Université Paris-Saclay, 91405 Orsay Cedex, France

Graphene nanoribbons (GNRs) have emerged as promising candidates for high-performance nanoelectronic devices due to their tunable energy band gaps resulting from lateral quantum confinement and edge effects. The recent development of on-surface synthesis has achieved various types of atomically precise GNRs, revealing fascinating electronic, magnetic, and mechanical properties. Their optical properties, on the other hand, remain largely unexplored. The intrinsic luminescence properties of atomically precise GNR remains remain to be addressed at single molecule level. Here, excitonic emission from atomically precise GNRs synthesized on a metal surface is probed using a scanning tunneling microscopy (STM) approach. A STM-based strategy to transfer the GNRs to a partially insulating surface is used to prevent light emission quenching of the ribbons by the metal substrate. Sub-nanometer resolved STM-induced fluorescence spectra reveal emission from localized dark excitons build upon the topological end states of the GNRs accompanying with a series of vibronic peaks. Our study provides a novel path to investigate the interplay between excitons, vibrons and topology in atomically precise graphene nanostructures.

O 2.7 Mon 12:00 CHE 89

Substrate induced magnetic alignment and magnetization dynamics of dimetallofullerene single-molecule magnets — •Tobias Birk[1], Fabian Paschke[2], Vivien Enenkel[1], Fupin Liu[3], Jan Dreiser[4], Vladyslav Romankov[4], Stanislav M. Avdoshenko[3], Alexey A. Popov[3], and Mikhail Fonin[1] — [1]Department of physics, University of Konstanz, 78457 Konstanz, Germany — [2]IBM Research Europe, 8803 Rüschlikon, Switzerland — [3]IFW Dresden, 01069 Dresden, Germany — [4]SLS, PSI, 5232 Villigen, Switzerland

Since several years, lanthanide based single-molecule magnets (SMMs) are in focus of a broad research community due to their record high blocking temperatures above 77 K [1]. However, surface supported SMMs lag behind in terms of blocking temperatures and relaxation times due to molecule-substrate interactions. Yet, for the surface-supported lanthanide dimetallofullerene SMMs blocking temperatures of up to 28 K and long relaxation times were reported [2]. Here, we study the effect of coupling to a metallic substrate on the electronic and magnetic properties of $\mathrm{Dy_2@C_{80}CH_2Ph}$ and compare those to our results for the graphene substrate [3,4]. A combination of scanning tunneling microscopy, -spectroscopy and X-ray absorption spectroscopy provides a detailed insight into the local electronic properties as well as magnetization dynamics of the studied SMMs.

[1] F.S. Guo *et al.* Science 362, 6421. [2] F. Liu *et al.* Nat. Commun. 10, 571 (2019). [3] F. Paschke *et al.* Adv. Mater. 2102844 (2021). [4] F. Paschke *et al.* Small 2105667 (2022)

O 2.8 Mon 12:15 CHE 89

Enantiospecific adsorption on a ferromagnetic surface at the single-molecule scale — •M.R. Safari[1], F. Matthes[1], K-H. Ernst[2], D.E. Bürgler[1], and C.M. Schneider[1] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich,52425 Jülich, Germany — [2]Molecular Surface Science Group, Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600, Dübendorf, Switzerland

The recently discovered effect of chirality-induced spin selectivity (CISS) not only enables spin-selective electron transport in organic molecules [1], but also offers a novel approach to chiral separation by exploiting the CISS-induced enantiospecific interaction of chiral molecules with perpendicularly magnetized substrates [2]. Using low-temperature spin-polarized scanning tunneling microscopy, we have investigated the enantiospecific adsorption of heptahelicene molecules on ferromagnetic Co bilayer islands [3,4]. High-resolution and spin-polarized STM images enable direct determination of the enantiomeric adsorption ratio R on oppositely magnetized Co islands. Statistical analysis of 748 molecules on 110 islands yields $R = 0.69 \pm 0.05$, which we attribute to different enantiospecific adsorption energies. The well-defined structural, electronic, and magnetic properties of the molecule-substrate systems make our results readily amenable to theoretical modeling that will hopefully shed light on the microscopic origin of enantiospecific adsorption on ferromagnetic surfaces. [1] R. Naaman et al., J. Phys. Chem. Lett. **3**, 2178 (2012); [2] K. Banerjee-Ghosh et al., Science **360**, 1331 (2018); [3] M.R. Safari et al., Nanomaterials **12**, 3281 (2022); [4] M.R. Safari et al., arXiv:2211.12976 (2022)

O 2.9 Mon 12:30 CHE 89

Clars goblet based J1 & J2 alternative heisenberg spin half chain — •Lin Yang — TU Dresden, Dresden, Germany

Spin-1/2 alternating-exchange Heisenberg chain has been intensively pursued for decades not only for understanding its underlying many-body physics but also for its great potential of realizing quantum computing and information. The existing candadites are limited in effective spin arrays embeded in three dimensional crystals, where the quasi-one dimensional spin system is inevitably affected by the cross talk between arrays and the spin-phonon coupling. Here, paradigmatic alternating-exchanging Heisenberg chains with spin-1/2 are realized in a designer graphene system using on-surface synthesis. The couplings: J1 = 38 meV, J2 = 23meV are determined by inelastic tunneling spectra, which is strong enough to support practical quantum operation.

O 2.10 Mon 12:45 CHE 89

CoPc on Ag(100): getting the most out of PEEM images — •Thorsten Wagner[1], Grazyna Antczak[2], Michael Györök[1], Anna Volokitina[1], Felix Marschner[1], Agata Sabik[2], Franciszek Gołek[2], and Peter Zeppenfeld[1] — [1]Johannes Kepler University, Institute of Experimental Physics, Surface Science Division, 4040 Linz, Austria — [2]University of Wrocław, Institute of Experimental Physics, 50-204 Wrocław, Poland

We use photoelectron emission microscopy (PEEM) and the Anderson method to study in situ the thin-film growth of cobalt-phthalocyanine (CoPc) on Ag(100) surfaces. Based on the Fowler-DuBridge theory, we were able to correlate the evolution of the mean electron yield acquired with PEEM for coverages up to two molecular layers of CoPc to the global work function changes measured with the Anderson method. For coverages above two monolayers, the transients measured with the Anderson method and those obtained with PEEM show different trends allowing us to determine the inelastic mean free path of the low-energy electrons while passing through the third layer of CoPc.[1] Already before (and during) the condensation of solid phases (2D islands or 3D crystallites), there is a dilute 2D gas phase consisting of individual molecules diffusing across the surface or clusters, which can not be resolved with PEEM. Therefore, we discuss, how image features below and above the resolution limit of a PEEM affect the mean electron yield and the (normalized) standard deviation.[2]

[1] Th. Wagner et al., ACS Appl. Mater. Interfaces 12 (2022), 23983–23989 [2] Th. Wagner et al., Ultramicrocopy 233 (2022), 113427

O 3: Metal Substrates: Adsorption and Reaction of Small Molecules I

Time: Monday 10:30–12:15 Location: CHE 91

O 3.1 Mon 10:30 CHE 91

A Nanocar and rotor in a molecule — •Kwan Ho Au-Yeung[1], Suchetana Sarkar[1], Tim Kühne[1], Oumaima Aiboudi[2], Dmitry A. Ryndyk[3,4], Roberto Robles[5,6], Nicolas Lorente[5,6], Franziska Lissel[2], Christian Joachim[7], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany, and Faculty of Chemistry and Food Chemistry, TU Dresden, 01062 Dresden, Germany — [3]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [4]Theoretical Chemistry, TU Dresden, 01062 Dresden, Germany — [5]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), 20018 Donostia-San Sebastián, Spain — [6]Donostia international physics center, 20018 Donostia-San Sebastian, Spain — [7]GNS & MANA Satellite, CEMES, CNRS, 29 rue J. Marvig, 31055 Toulouse, France

Depending on its adsorption conformation on the Au(111) surface, a zwitterionic single molecule machine works in two different ways under STM voltage pulses: It is a unidirectional single molecule-rotor while anchoring on the surface; It is a fast-drivable molecule-vehicle (nanocar) while physisorbed. By tuning the molecular coverage, the conformation of the molecule can be selected as a rotor or a nanocar. The movement triggered by inelastic tunneling excitation is investigated under the same experimental conditions for the unidirectional rotation of the rotor and the directed movement of the nanocar.

O 3.2 Mon 10:45 CHE 91

Controlling the Switching of Azobenzene Derivatives on Graphite-Air Interface — •Thiruvancheril G. Gopakumar[1], Khushboo Yadav[1], Hariom Birla[1], Showkat H. Mir[2], Thomas Halbritter[3], Alexander Heckel[3], and Jayant K. Singh[2] — [1]Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India — [2]Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur 208016, India — [3]Institute for Organic Chemistry and Chemical Biology, Goethe-University Frankfurt, Max-von-Laue-Str. 9, 60438 Frankfurt, Germany

The trans isomer of azobenzene (AB) and its derivatives is the most abundant under equilibrium-thermodynamical conditions and is known to switch between its trans and cis states when triggered by light and electrons/holes on graphite.[1] In this work, we show that AB derivatives are switching between two cis states (cis, cis') when electrons/holes induced switching is performed on a cis dominant non-equilibrium initial condition at HOPG-air interface. The switching efficiency in the cis adlayer is several folds higher than that in the trans adlayer. This is related to the low switching barrier for cis-cis' switching compared to that of trans-cis switching as revealed by density functional theory (DFT) calculations.[2]

1) K. Yadav, S. Mahapatra, T. Halbritter, A. Heckel, T. G. Gopakumar, J. Phys. Chem. Lett., 2018, 9, 6326-6333. 2) K. Yadav, H. Birla, S. H. Mir, T. Halbritter, A. Heckel, J. K. Singh, T. G. Gopakumar, Appl. Surf. Sci. 2023, 612, 155747

O 3.3 Mon 11:00 CHE 91

STM-induced ring closure of vinylheptafulvene molecular dipole switches on Au(111) — •Suchetana Sarkar[1], Kwan Ho Au-Yeung[1], Tim Kuehne[1], Oumaima Aiboudi[2], Dmitry A. Ryndyk[3,4], Thomas Heine[4], Franziska Lissel[2,4], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Leibniz Institute of Polymer Research, 01069 Dresden, Germany — [3]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [4]Faculty of Chemistry and Food Chemistry, TU Dresden, 01062 Dresden Germany

Dihydroazulene/vinylheptafulvene pairs are known as molecular dipole switches that undergo a ringopening/- closure reaction by UV irradiation or thermal excitation. We show that the ring-closure reaction of a single vinylheptafulvene adsorbed on the Au(111) surface can be induced by voltage pulses from the tip of a scanning tunneling microscope. This cyclization is accompanied by the elimination of HCN, as confirmed by simulations. Post the ring closure reaction, lateral movement induced via voltage pulses from the STM tip shows a different response. This behaviour is discussed by comparing the dipole moment and the charge distribution of the open and closed forms on the surface.

O 3.4 Mon 11:15 CHE 91

Surface segregation of PdAu(111) in reactive gas environments from ab initio thermodynamics — •Olga V Vinogradova, Vanessa J Bukas, and Karsten Reuter — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Catalytic properties of alloys are largely determined by the specific chemical composition at the surface. Differences in composition between surface and bulk regions depend intricately on both the parent metals and surrounding gas-phase environment. While a non-reactive environment is expected to induce surface segregation of the more noble alloy component, a reactive environment such as oxygen often favors the more active component at the surface. Using ab initio thermodynamics, here we explore the structure and composition of the PdAu(111) alloy surface in oxygen, nitrogen, and carbon containing environments. An exhaustive, yet systematic, search of the available phase-space shows the segregation profile in an oxygen atmosphere to follow the anticipated picture described above. Unlike oxygen, however, carbon at low coverages burrows deeper into the alloy substrate without first the adsorbate-induced segregation of Pd at the surface. A nitrogen environment induces an intermediate behavior to oxygen and carbon where the nitrogen atoms first favor either surface or subsurface sites depending on the detailed metallic composition profile.

O 3.5 Mon 11:30 CHE 91

Atomistic investigations on the effect of vibrational excitation on O$_2$ adsorption on Pt surfaces — •Simon Homann, Björn Kirchhoff, and Timo Jacob — Institute of Electrochemistry, Ulm University, D-89081 Ulm

Platinum is considered an excellent model system for surface studies and is also an important heterogeneous catalyst. Combined with non-thermal plasmas, many studies found an improvement in turn-over frequency compared to thermal catalysis with the non-excited gas phase. One possible contender towards an explanation of this is the interaction of the vibrationally excited molecules in the plasma with the metal surface. As a first proof of concept, we present in this study Born-Oppenheimer molecular dynamics simulations of vibrationally excited Oxygen on low-indexed Platinum surfaces using a reactive force field (ReaxFF). The vibrational density of states simulated this way is in agreement with typical results obtained, *e.g.* from kinetic modeling of the plasma afterglow. The higher vibrational energy leads to an altered adsorption behavior in terms of dissociation and preferred adsorption positions, as well as changes in surface morphology.

O 3.6 Mon 11:45 CHE 91

Fluctuating nature of CO adlayer structures on metal surfaces — •Sung Sakong and Axel Gross — Ulm University, Ulm, Germany

The dynamics of atomic and molecular adlayers on surfaces is an critical issue in heterogeneous catalysis and electrocatalysis as it determines how reaction partners can meet on the catalyst surfaces. The adlayer formation influences the performance of catalysts and the structure of the electric double layer. Recently, video scanning tunneling microscope (V-STM) experiments have demonstrated the influence of the CO adlayer dynamics on oxygen diffusion on Ru(0001) [1,2] and the dynamical nature of a CO monolayer on Pt(111) [3]. We will present microscopic pictures of CO adlayer fluctuations on Ru(0001) and Pt(111) based on density functional theory (DFT) calculations and kinetic Monte Carlo (kMC) simulations. The calculations demonstrate how local disorder can lower the adsorption energy of a CO adlayer. We will particularly demonstrate the importance of the so-called door opening mechanism for oxygen diffusion on a CO-covered surface [1,2] and the dynamical nature of CO adlayers [3] by comparing DFT-based simulations with V-STM experiments.

[1] A. Henß *et al.*, Science **363**, 715 (2019).
[2] S. Sakong *et al.*, J. Phys. Chem. C **124**, 15216 (2020).
[3] J. Wei *et al.*, Angew. Chemie. Int. Ed. **59**, 6182 (2020).

O 3.7 Mon 12:00 CHE 91

Self-assembly and dehydrogenation reactions of borazine on

Ag(111) — •Tobias Weiss[1], Aleksandr Baklanov[1], Georg S. Michelitsch[2], Martin Schwarz[1], Manuela Garnica[1], Karsten Reuter[3], and Willi Auwärter[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Laboratoire des Solides Irradiés, École Polytechnique, France — [3]Chair of Theoretical Chemistry, Technical University of Munich, Germany

Borazine ($B_3N_3H_6$), is a prominent precursor for the growth of hexagonal boron nitride (*h*BN) on metal supports [1]. With monolayer *h*BN playing an important role in the field of 2D-materials, borazine adsorption, assembly and decomposition on surfaces is a topic of interest. Space-averaging studies revealed flat or tilted adsorption geometries on different substrates depending on their catalytic activity [2,3].

Here, we provide unprecedented real-space insight into adsorbed borazine molecules and their on-surface chemistry in ultra-high vacuum. This scanning tunneling microscopy investigation of the self-assembly of borazine on Ag(111) reveals a highly regular, porous hexagonal phase or a dense packed structure, depending on exposure. Furthermore, tip-induced dehydrogenation reactions of single molecules result in a tilted adsorption geometry. Complementary density functional theory calculations were performed to comprehensively characterize potential reaction products and adsorption configurations.

[1] W. Auwärter, Surf. Sci. Rep., 2019, 74, 1-95
[2] R. Simonson, Surf. Sci., 1991, 254, 29-44
[3] L. Haug, Phys. Chem. Chem. Phys., 2020, 22, 11704

O 4: Tribology: Surfaces and Nanostructures

Time: Monday 10:30–12:30 Location: GER 37

O 4.1 Mon 10:30 GER 37

High throughput first-principle prediction of interfacial adhesion energies in metal-on-metal contacts — Paolo Restuccia, •Margherita Marsili, and Maria Clelia Righi — Department of Physics and Astronomy, University of Bologna, 40127 Bologna, Italy

Adhesion energy ultimately dictates the mechanical behavior and failure of interfaces. As natural and artificial solid interfaces are ubiquitous, it represents a key quantity in a variety of fields, from geology to nanotechnology. An *ab-initio* determination of adhesion energies is crucial because the specific atomistic details of the interface primarily determine the strength of adhesion, but, especially for heterogeneous interface is challenging, as computations can be very expensive. We performed the high-throughput DFT determination of the adhesion energy of around a hundred metallic heterostructures, ranging from transition to noble metals [1]. We identified general trends confirming that adhesion energies can be reasonably well inferred from the knowledge of the surface energies of the two interface constituents. Finally, by using a machine learning approach, we obtained a simple analytical expression for predicting the adhesion energy from the intrinsic properties of the two heterostructure constituents alone, which can prove useful for avoiding expensive supercell calculations. These results are part of the SLIDE project funded by the European Research Council under the Horizon 2020 research and innovation program (Grant agreement No. 865633). [1] P. Restuccia et al. *High throughput accurate prediction of interfacial adhesion energies in metal-on-metal contacts* submitted to npj Computational Materials (2022)

O 4.2 Mon 10:45 GER 37

Nanoscale Friction across the First Order Charge Density Wave Phase Transition of 1T-TaS$_2$ — Wen Wang[1], •Dirk Dietzel[2], and Andrè Schirmeisen[2] — [1]School of Mechanical Engineering, Southwest Jiaotong University, Chengdu, China — [2]Institute of Applied Physics, Justus Liebig University Giessen, Giessen, Germany

In material science, analyzing phase transitions is a fundamental way to understand material properties and their changes on the atomic level. At the same time, phase transition materials are intriguing model systems for nanotribology, where well-defined transformations can occur if a specific control parameter, like e. g. temperature, changes. On one hand, varying friction between tip and sample can be linked to the specific properties of different phases. On the other hand, during the phase transition localized mechanical probing of the surface can allow for a direct coupling to the reorganization of the material as was recently demonstrated for the case of 1T-TaS$_2$ [1]. However, previous experiments did not allow for an in-depth analysis of the influence of crucial parameters like sliding velocity and normal force on the process of local nucleation. This was now done by friction force microscopy on 1T-TaS2 for different stationary temperatures across the charge density wave phase transitions. Our results corroborate an anticipated mechanism, where the AFM-tip gradually induces local transformations of the material close to the spinodal point in a thermally activated and shear assisted process until the surface is fully 'harvested'.

[1] Panizon et al., New Journal of Physics 20, 023033 (2018).

O 4.3 Mon 11:00 GER 37

Kinetic nanoscale friction on van der Waals heterostructures — •Bartosz Szczefanowicz[1], Zhao Liu[1], Joao Marcelo J. Lopes[2], Antony George[3], Ziyang Gan[3], Andrey Turchanin[3], Alexander Rothstein[4], Christoph Stampfer[4], and Roland Bennewitz[1] — [1]INM - Leibniz Institute for New Materials, Saarbrücken, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [3]Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena, Germany — [4]JARA-FIT and 2nd Institute of Physics A, RWTH Aachen University, 52074 Aachen, Germany

2D materials exhibit exceptional tribological properties due to their weak normal-to-plane interactions. Friction Force Microscopy (FFM) demonstrated that the microscopic processes underlying friction can be tuned by application of high contact pressure [1] or by combining different 2D materials into van der Waals heterostructures [2].

Samples of MoSe$_2$/hBN and graphene/hBN were prepared by the exfoliation technique. Sample of MoS$_2$/graphene was produced by thermal decomposition of SiC(0001), followed by direct growth of MoS$_2$ by Chemical Vapor Deposition (CVD). Friction forces were measured on those heterostructures in FFM experiments in ultrahigh vacuum as function of normal load and electric bias. We will discuss the results in terms of atomic potential corrugation, bending rigidity of 2D heterostructures, and bias-induced electrostatic attraction.

[1] T. Filleter, and R. Bennewitz, Phys. Rev. B, 81, 2010, 155412
[2] M. R. Vazirisereshk, et al., Nano Lett., 19, 2019, 5496-5505

O 4.4 Mon 11:15 GER 37

Temperature Dependent Wear Effects on the Nanometer Scale — •Jennifer Konrad, Dirk Dietzel, and Andre Schirmeisen — Institute of Applied Physics, Justus-Liebig University Giessen, 35392 Giessen, Germany

On the nanoscale, the temperature dependence of friction as observed by friction force microscopy is a well-known phenomenon that can often be described by the thermally activated Prandtl Tomlinson Model. Similarly, nanoscale wear is also often anticipated as a thermally activated and shear assisted process, which results in a temperature dependence, where the overall wear rate increases with temperature [1]. However, this behavior can change when the effects of interfacial bond formation and breaking have to be taken into consideration. Surprisingly, lower temperatures can then result in higher wear rates as will be demonstrated by temperature dependent wear experiments performed for different interfaces involving silica and diamond surfaces. This behavior can phenomenologically be explained by considering shear assisted bond formation, which leads to a higher number of interfacial bonds formed at lower temperatures [2]. By straining this larger number of bonds during scanning an increased wear rate at low temperatures is then caused, even if the energy barrier for bond breaking is lower than for the removal of adjacent surface atoms.

[1] W. Wang, D. Dietzel, and A. Schirmeisen, Phys. Rev. Lett. 126, 196101 (2021).

[2] M. Vorholzer et al., Physical Review X 9, 041045 (2019).

O 4.5 Mon 11:30 GER 37

Rewritable friction on Nitrogen-doped graphene moiré superstructures — •Shuyu Huang[1,2], Antoine Hinaut[2], Yiming Song[2], Sebastian Scherb[2], Gema Gnavarro[2], Thilo Glatzel[2], Yunfei Chen[1], and Ernst Meyer[2] — [1]Jiangsu Key Laboratory for Design and Manufacture of Micro-Nano Biomedical Instruments, School of Mechanical Engineering, Southeast University, Nanjing

211189, China — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Graphene, as typical atomically-thin solid lubricant with potential applications in micro- and nano-electromechanical systems (MEMS/NEMS), has been extensively investigated on its nanotribological properties. In the present work, we compare the frictional properties between pristine graphene and modified graphene, showing that atomic-scale friction can be significantly altered by Nitrogen doping-induced modification, then it can be recovered after tip rubbing. Specifically, C60 nano-flakes are deposited as a mask on graphene/Ir (111) surface by thermal evaporation. The sample is then exposed to a nitrogen radical flux produced by a remote RF plasma source. After thermal annealing, to desorb C60 molecules, both nanopatterned modified graphene and pristine graphene, located below former C60 islands, surface is obtained simultaneously. By the means of high-resolution ultrahigh vacuum atomic force microscopy, the topography of surface with two different regions are characterized and discussed in non-contact mode and friction force variation is measured in contact mode.

O 4.6 Mon 11:45 GER 37

Atomic friction over bonds: Impact of the chemical neighbourhood — •Lukas Hörmann[1], Johannes J. Cartus[1], Alfred J. Weymouth[2], and Oliver T. Hofmann[1] — [1]Institute of Solid State Physics, Graz University of Technology, Graz, Austria — [2]Universität Regensburg, Regensburg, Germany

Friction causes a significant amount of energy loss in any moving mechanical device. Given the trend toward the miniaturisation of devices, studies of the fundamental mechanisms governing friction at the atomic scale become ever more important. At this scale, friction is governed by electronic and phononic excitations as well as by the potential energy surface (PES) at the interface.

We computationally investigate these mechanisms on the example of a CO-tip of a lateral force microscope oscillating above a PTCDA monolayer on Cu(111). Our investigation combines ab-initio electronic structure methods with machine-learning algorithms to predict highly accurate PESs and to estimate frictional energy dissipation. We gauge the dependence of frictional energy dissipation on the local chemical environment, i.e. the location of the CO-tip above the surface during the friction measurement. Moreover, we investigate how the oscillation direction and the stiffness of the CO-tip affect friction. Hereby we study the role of quantum-mechanical interactions by comparing our results to friction estimates based on a Lennard-Jones potential as well as experimental measurements. Finally, we investigate frictional energy dissipation channels by studying how the movement of the CO-tip may be damped as a result of electronic friction.

O 4.7 Mon 12:00 GER 37

Quantum-mechanically enhanced water flow in subnanometer carbon nanotubes — •Alberto Ambrosetti, Giorgio Palermo, and Pier Luigi Silvestrelli — Dipartimento di Fisica e Astronomia, Università degli Studi di Padova, via Marzolo 8, 35131, Padova, Italy

Water-flow in carbon nanotubes (CNT's) starkly contradicts classical fluid mechanics, with permeabilities that can exceed no-slip Haagen-Poiseuille predictions by two to five orders of magnitude. Semiclassical molecular dynamics accounts for enhanced flow-rates, that are attributed to curvature-dependent lattice mismatch. However, the steeper permeability-enhancement observed experimentally at nm-size radii remains poorly understood, and suggests emergence of puzzling non-classical mechanisms. Here we address water-CNT friction from a quantum-mechanical perspective, in terms of water-energy loss upon phonon excitation. We find that combined weak water-phonon coupling and selection rules hinder water-CNT scattering, providing effective protection to water super flow, whereas comparison with a semiclassical theory evidences a friction increase that can exceed the quantum-mechanical prediction by more than two orders of magnitude. Quasi-frictionless flow up to sub-nm CNT's opens new pathways towards minimally-invasive trans-membrane cellular injections, single-water fluidics and efficient water filtration.

O 4.8 Mon 12:15 GER 37

Screw-like beetle joints and their tribological features — •Cornelia F. Pichler[1], Richard Thelen[1], Thomas van de Kamp[2], and Hendrik Hölscher[1] — [1]Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology, Karlsruhe, Germany

Understanding and finally mimicking lubricants in the joints of various insects promises environmentally friendly alternatives for mineral-oil-based lubricants. The compactness of the insect joints and the tiny quantities of their respective lubricants make it challenging to analyze their frictional properties. In my work, I characterize lubricants directly in dissected screw-like beetle joints by lateral force measurements with the atomic force microscope (AFM). This approach gives insight into the frictional properties of the lubricant in its natural form as well as the functional structure found in the joints. In addition to lubricant films, we also observe microstructures which suggest that beetles advance frictional properties of their joints by a sophisticated combination of surface structure and lubrication.

O 5: Focus Session: Ion Beam Interaction with Surfaces and 2D Materials I

Ion beam techniques are an important tool in surface science and nanotechnology in terms of surface composition analysis as well as tailoring of surface properties. Recent important developments took place using ultra-low energy ion implantation to introduce foreign atoms into 2D material lattices or triggering self-organization mechanisms to form large-scale ordered crystalline surface structures. This focus session brings international specialists in the connecting fields of ion physics and surface science together to discuss recent progress to our fundamental understanding of ion-surface interactions as well as pathways towards new applications for emerging material classes.

Organizer: Richard Arthur Wilhelm (TU Wien)

Time: Monday 10:30–13:00 Location: GER 38

Topical Talk O 5.1 Mon 10:30 GER 38

Highly charged, slow and swift ions interacting with surfaces and 2D materials — •Marika Schleberger — Fakultät für Physik, Universität Duisburg-Essen and CENIDE

Ion beams are a proven, versatile, and efficient tool for material modification and in particular for defect engineering. An ion stores its energy in the form of kinetic (E_{kin}) and so-called potential energy (E_{pot}), the latter corresponding to the energy required to create its respective charge state. At low velocities, the energy deposition is based on elastic collisions leading to linear sputtering cascades or collision peaks in the volume of the material, and ultimately to the emission of atoms. At higher kinetic energy, electronic excitations and ionizations are dominant. The release of potential energy again occurs via electronic processes that can also lead to the emission of atoms from the target material. By adjusting these two parameters, E_{pot} and E_{kin}, one can in principle fine-tune the nature of the interaction and thus the corresponding material changes. However, the basic mechanisms of defect formation through electronic excitation have not yet been clarified. We have introduced 2D materials as target material for the study of ion-solid-interactions. Due to their well-defined thickness, the flexible preparation and last but not least the wide range of available materials, they are an ideal target material for our task. We have studied the interaction of ions of different types with surfaces and 2D materials and I will present key results.

O 5.2 Mon 11:00 GER 38

Model for Nanopore Formation in Two-Dimensional Materi-

als by Impact of Highly Charged Ions — •A. S. Grossek, A. Niggas, R. A. Wilhelm, F. Aumayr, and C. Lemell — TU Wien

Experiments of highly charged ions (HCI) on 2D-materials have shown that HCIs extract numerous electrons from the 2D target. This interaction has shown to lead to nanopore formation in materials such as monolayer MoS_2 while single layer graphene remains structurally intact. One hypothesis proposed for the cause of nanostructuring of these materials is charge build up by hole charges in the target, which -depending on material charge conductivity- may sustain sufficiently long in order to lead to structural damage of the target atoms. We study this hypothesis of nanostructuring by HCI impact on 2D-materials via molecular dynamics simulations. The charge transfer from target to HCI is well described by the classical-over-the-barrier model, of which a simplified version is implemented into the simulation. Charge conduction in the target is modelled by charge hopping with a hopping time t_h between lattice sites. Our 2D lattice is simulated by a Stillinger-Weber potential with parameters fitted to reproduce graphene. We study different materials by respectively adjusting the hopping time t_h (conductivity) of the graphene lattice in the simulation. After the simulation kinetic and potential energies of the individual target atoms are evaluated to determine if a pore has formed. Our simulation is able to qualitatively reproduce experimental results showing pore formation efficiencies and pore sizes to be dependent on initial HCI charge state and conductivity of the material.

O 5.3 Mon 11:15 GER 38

Charge-state-enhanced ion sputtering of metallic gold nano islands — •Gabriel L. Szabo[1], Benedykt R. Jany[2], Helmut Muckenhuber[1], Anna Niggas[1], Markus Lehner[1], Arkadiusz Janas[2], Paul S. Szabo[3], Antony George[4], Ziyang Gan[4], Andrey Turchanin[4], Franciszek Krok[2], and Richard A. Wilhelm[1] — [1]TU Wien, Institute of Applied Phyiscs, 1040 Vienna, Austria, EU — [2]Jagiellonian University, Institute of Physics, 30-348 Kraków, Poland, EU — [3]University of California, Space Sciences Laboratory, Berkeley 94720, USA — [4]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena, Germany, EU

Irradiation of certain targets with slow highly charged ions (HCIs) can trigger phase transitions or nano-structure formation. The main driving force for these processes is the electronic excitation of the target's electronic sub-system in close proximity of the impact triggered by the ion neutralization. Subsequent electron-phonon coupling mediates lattice heating of the target. So far charge state dependent erosion of metallic surfaces was not unambiguously shown. The potential energy stored in the HCI dissipates quickly before a transfer to the target's atomic lattice can take place. By reducing the size of the target down to the nanometer regime, geometric confinement might prevent free electrons of the target to dissipate the electronic excitations on the fs time-scale. In this work we irradiated gold nano islands with Xe^{q+} (q=1,18,25,32,40) with a constant kinetic energy of 180 keV, which results in an erosion of the islands that is strongly enhanced by the potential energy deposition.

Topical Talk O 5.4 Mon 11:30 GER 38

A contactless single-step process for simultaneous nanoscale patterning and cleaning of large-area graphene — •Tuan Tran — Department of Physics and Astronomy, Uppsala University, Sweden

In this talk, we will present a contactless single-step process for structuring self-supporting graphene with customizable patterns and over large areas. Using energetic ions passing through a suspended mask with through-hole nanopatterns, we can deterministically structure the graphene with a minimum feature size down to 15 nm, comparable to what can be achieved with focused ion beam techniques. Our process, however, instead uses a broad parallel beam with no stringent requirement on the beam focusing, and hence enables a contactless approach. Neither, any chemicals and coating layers are necessary, substantially reducing the amount of contamination which might otherwise occur using other lithographic methods. In addition to the structuring capability, we found that the method can simultaneously render the graphene cleaner. The areas surrounding the direct ion impacts are significantly cleaned from the initial contamination which commonly are remnants from the transferring process of the graphene. We will explain the mechanism leading to such cleaning effect. Finally, selective area electron diffraction were used for detailed characterization of the graphene lattice after ion irradiation with and without the mask at different doses and temperatures. These diffraction data are necessary for understanding the creation and annihilation of defects and the possible role of the contamination on self-healing and stabilization of the graphene lattice.

O 5.5 Mon 12:00 GER 38

chemical etching of 2D materials — •Mitisha Jain, Silvan Kretschmer, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

Transmission electron microscopes are used for imaging 2D materials to the resolution of single atoms. On the other hand, the imaged material gets damaged (modified by the beam) quite easily. Hence, the information about the damage done by the beam are important for proper imaging. Different channels of damage construction such as knock-on, ionization (excitation), chemical etching (e.g. adatoms) have been determined. In this study, the knock-on threshold energies for graphene (C), h-BN (B and N) and MoS2 (S) materials in the presence of adsorbed adatoms (H, C, N, O) on the surface are calculated in the framework of spin-polarized density functional theory. From the preliminary results, we found that when an adatom is adsorbed, the threshold energies are reduced by 2-3 eV compared to pristine systems. Further, we consider the additional effect of electronic excitation on the threshold energies in combination with adsorbed adatoms. The displacement cross-section under the electron beam are assessed employing the McKinley-Feshbach formalism allowing to compare different channels of damage creation.

O 5.6 Mon 12:15 GER 38

Influence of the swift heavy ions' charge state on pore creation in single-layer MoS_2 — •Yossarian Liebsch[1], Lukas Madauss[1], Henning Lebius[2], Abdenacer Benyagoub[2], Clara Grygiel[2], Radia Rahali[2], Rajendra Singh[3], Jani Kotakoski[3], and Marika Schleberger[1] — [1]University Duisburg-Essen, Duisburg, Germany — [2]CIMAP/GANIL, Caen, France — [3]University Vienna, Vienna, Austria

The initial charge state of a swift heavy ion is usually of no special interest when discussing the interaction of the ion with a bulk target. This is due to the potential energy being small in comparison to the kinetic energy of the ion and due to the equilibrium charge the ion accumulates within a few nanometers after it enters the material. However, in single-layer materials the travelling distance is less than the typical distance needed to establish the equilibrium charge state. Hence, we try to investigate the influence of the charge state of the ions on the defect formation in MoS_2. This is done by irradiating single-layers with swift heavy ions of different charge states. For this experiment we chose 6.6 MeV/u Xe ions with charge states ranging from +41 to +48. Evaluation of the effect on the material is done by analyzing the pore radii and creation efficiencies with STEM-HAADF. With this experiment we aim to shed light onto the fundamental processes and interactions between ultra thin materials and swift heavy ions as well as quantifying the influence of the charge state on the stopping power in single-layered materials.

O 5.7 Mon 12:30 GER 38

Spectroscopic and microscopic analysis of ion-induced modifications in 2D materials — •Carolin Frank[1], Lucia Skopinski[1], Lars Breuer[1], Jennifer Schmeink[1], Lukas Kalkhoff[1], Stephan Sleziona[1], Ulrich Hagemann[2], and Marika Schleberger[1] — [1]University of Duisburg-Essen, Faculty of Physics and CENIDE, 47057 Duisburg, Germany — [2]University of Duisburg-Essen, CENIDE, ICAN, 47057 Duisburg, Germany

In this contribution we present results concerning modifications induced by xenon- and gold-ions in two-dimensional molybdenum disulfide exfoliated on gold including Raman spectroscopy, X-ray photoelectron spectroscopy and friction force microscopy. Irradiations at the target station HICS, located at the University of Duisburg-Essen, as well as at the target stations MSS@CRYRING and M1-Branch, both located at the GSI Helmholtzzentrum für Schwerionenforschung, were implemented with slow, highly charged ions as well as with swift heavy ions, which differ from each other regarding their charge state and their kinetic energy.

A focus will be given to the impact of both the kinetic and potential energy of the ions on modifications of the molybdenum disulfide and also on the size of ion-induced defects. Based on the results of friction force microscopy it is shown for the first time that the impact of the potential energy of the swift ions regarding generation of defects in 2D materials is significantly larger than the impact of the kinetic energy. Additionally, results regarding interaction between the gold substrate and the molybdenum disulfide will be discussed.

O 5.8 Mon 12:45 GER 38

Manipulation of the electrical and memory properties of MoS_2 field-effect transistors by highly charged ion irradiation — •Stephan Sleziona[1], Aniello Pelella[2], Enver Faella[2], Osamah Kharsah[1], Lucia Skopinski[1], André Maas[1], Yossarian Liebsch[1], Antonio Di Bartolomeo[2], and Marika Schleberger[1] — [1]Fakultät für Physik und Cenide, Universität Duisburg-Essen, Lotharstraße 1, 47057 Duisburg — [2]Physics Department, University of Salerno, 84084 Fisciano, Salerno, Italy

Molybdenum disulfide (MoS_2) is a semiconductor that develops a direct bandgap of 1,8 eV when its thickness is reduced to the monolayer limit and is therefore a suitable 2D material for applications in optoelectronic devices. MoS_2 field-effect transistors (FET) in particular exhibit a hysteresis in their transfer characteristics, which can be utilized to realize a 2D memory device. This hysteresis is generally attributed to adsorbates or defects either in the MoS_2 lattice or in the underlying substrate. We fabricated MoS_2 FETs on SiO_2/Si substrates and irradiated these devices with Xe^{28+} ions at a kinetic energy of 180 keV to deliberately introduce defects and modify their electrical and hysteretic properties. We evaluate different electrical properties before and after the irradiation and find clear influences of the irradiation e.g., on the conductivity and charge carrier mobility of the devices. Significantly reduced n-doping and a well-developed hysteresis can be measured after irradiation. We utilize this hysteresis to demonstrate the use of the MoS_2 FET as a memory device, which has remarkably longer relaxation times ($\approx$ minutes) compared to previous works.

O 6: New Methods: Experiments and Theory

Time: Monday 10:30–13:00 Location: GER 39

O 6.1 Mon 10:30 GER 39

A Newly Developed IRAS System to Investigate Adsorbates on Metal-Oxide Single Crystal Surfaces — •David Rath, Jiri Pavelec, Ulrike Diebold, Michael Schmid, and Gareth S. Parkinson — Institute of Applied Physics, TU Wien, Austria

The IRAS system GRISU (GRazing incident Infrared absorption Spectroscopy Unit) was developed to investigate adsorbates on metal oxide single crystals in the research field of single-atom catalysis [1]. It combines the commercially available FTIR spectrometer Bruker Vertex 80v with an UHV chamber [2]. The compact design requires only one CF150 port for the main optical components, features five mirrors for beam guidance placed in HV and UHV environment and optimises the system's performance, flexibility, and usability. The result is a small controllable focal-spot diameter (max. 3 mm) on the sample, motorised optical components, and an aperture limiting the incidence angle range (variable, 49° to 85°) on the sample. Based on ray tracing results and preliminary intensity measurements, the system shows up to 10× higher intensities compared to a commercial system with two parabolic mirrors with a focal length of 250 mm. First IR spectra measured with the recently installed IRAS measurement system will be shown.

[1] G. S. Parkinson, Catal. Lett. 149, 1137 (2019)

[2] J. Pavelec, et al., J. Chem. Phys. 146, 014701 (2017).

O 6.2 Mon 10:45 GER 39

Insights on the Liquid/vacuum interface of ionic liquids by ARXPS and UHV Pendant Drop — Ulrike Paap, •Afra Gezmis, Florian Maier, and Hans-Peter Steinrück — Friedrich-Alexander Universität, Erlangen, Germany

Ionic liquids (ILs) are characterized by a low melting point and a low vapor pressure. Many ILs exhibit high gas solubility along a high chemical and thermal stability. Such properties are beneficial in many areas such as gas absorbents, refrigerants, lubricants, antistatics and surfactants. The low vapor pressure of ILs opens the possibility to investigate them under ultra-high vacuum (UHV) conditions. In this context, angle-resolved X-ray photoelectron spectroscopy (ARXPS) has already proven to be a particularly powerful tool. We now combine information on the surface composition derived from ARXPS and measurements of the surface tension performed under ultraclean conditions with our new pendant drop setup, which operates in UHV. Our results allow for a deeper understanding of enrichment and molecular orientation processes at the outermost surface of these systems on the microscopic and the macroscopic scale. This work was supported by the Collaborative Research Center (CRC) 1452: Catalysis at Liquid Interfaces.

O 6.3 Mon 11:00 GER 39

Kintetic In Situ Synthesis (KISS) technique of large-area 2D materials exfoliation — •Antonija Grubisic-Cabo[1,2], Matteo Michiardi[3], Charlotte E. Sanders[4], Marco Bianchi[5], Davide Curcio[5], Dibya Phyual[2], Magnus H. Berntsen[2], Qinda Guo[2], and Maciej Dendzik[2] — [1]University of Groningen, Netherlands — [2]KTH, Sweden — [3]University of British Columbia, Canada — [4]Central Laser Facility, UK — [5]Aarhus University, Denmark

Two-dimensional (2D) materials provide an extremely rich platform to investigate novel quantum phenomena and to design nanostructures with desired functionalities. Some of the key techniques employed in studies of 2D materials, such as photoemission spectroscopy, have stringent requirements for the quality, sample size and cleanliness of the surface. Fulfilling these conditions using a standard mechanical exfoliation in a glove box is often problematic. Here, we present a novel method for in situ exfoliation of 2D materials performed directly in ultra-high vacuum, which yields large flakes of excellent crystallinity and purity. In our experiments, multiple semicondicting and metallic transition metal dichalcogenides were exfoliated onto Au, Ag and Ge substrates, showing the versatility of the technique, and characterised by angle resolved photoemission spectroscopy. Importantly, the proposed method is straightforward, simple, and does not require any specialised equipment. This technique is ideally suited for the electronic structure research of air-sensitive 2D materials since the sample preparation process happens entirely in ultra-high vacuum.

O 6.4 Mon 11:15 GER 39

Two new methods for the analysis of TPD data — •Michael Schmid, Gareth S. Parkinson, and Ulrike Diebold — Institute of Applied Physics, TU Wien, Austria

Temperature programmed desorption (TPD) is the most common experimental technique for obtaining the binding energies of adsorbates. TPD data are usually analyzed using the Polanyi–Wigner equation; this is far from straightforward. We present two new methods, based on equilibrium thermodynamics, bypassing the use of the Polanyi–Wigner equation or transition state theory: In the case of all adsorption sites being equivalent, the adsorption energy can be directly calculated from the desorption temperature, the width of the TPD peak, the sticking probability (at the desorption temperature), and thermodynamic data [1]. This "magic formula" is remarkably robust; in many cases even wrong assumptions about the desorption order or the presence of a distribution of adsorption energies lead to negligible errors. In more complex cases, with a distribution of adsorption energies, we show that TPD spectra are approximately given by a convolution integral. We present a method (and computer program) for TPD inversion, i.e, the determination of the energy distribution from a single TPD spectrum at saturation coverage [1]. Although this method is derived for the case of non-interacting adsorbates, we argue that it is a good approximation in cases of short-range repulsion and it can also reveal (though not quantitatively analyze) the presence of attractive interactions between adsorbates.

[1] M. Schmid et al., doi:10.1021/acsphyschemau.2c00031 (2022)

O 6.5 Mon 11:30 GER 39

Surface-Sensitive Spectroscopy from First Principles — •Yair Litman[1,2], Jinggang Lan[3], Kuo-Yang Chiang[2], Venkat Kapil[1], Yuki Nagata[2], and David Wilkins[4] — [1]University of Cambridge, Cambridge, United Kingdom — [2]MPI for Polymer Research, Mainz, Germany — [3]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [4]Queen's University Belfast, Belfast, United Kingdom

Our current understanding of the structure and dynamics of aqueous interfaces at the molecular level has grown substantially in the last decades due to an increasing synergy between experimental measurements and atomistic simulations. However, the latter are either based on empirical force field models, which are neither suitable to describe bond breaking and formation nor systems with complex electronic structure, or on *ab initio* calculations which due to their computational cost cannot be statistically converged. In this work, we overcome all these limitations by combining high-dimensional neural network potentials with symmetry-adapted Gaussian process regression [1] to simulate the sum-frequency generation (SFG)[2] spectra of the water-air interface with *ab initio* accuracy. We obtain a good agreement with last-generation experiments and show how these models can in principle be improved systematically towards exact results. Overall, the machinery presented in this work paves the way for the modelling of surface-sensitive spectroscopy of complex interfaces. [1] V. Deringer, *et al.*, Chem. Rev. **16**, 121 (2021) [2] A. Morita, J. Hynes, J. Phys. Chem. B **106**, 673 (2002).

O 6.6 Mon 11:45 GER 39

Artifical Neural Network based Interatomic Potentials to Describe Laser-Excited Materials — •Bernd Bauerhenne, Pascal Plettenberg, and Martin E. Garcia — Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Femtosecond laser pulses create a transient state with hot electrons at temperature Te and cold ions, in which ultrafast nonthermal effects occur. Later, the decay of this state due to electron-phonon interactions gives rise to ultrafast effects of more thermal character. Quantum mechanical methods like Te-dependent density functional theory (DFT) allow a precise description of the non-thermal state with hot electrons. However, simulations of laser material interactions at surfaces on experimentally relevant sizes require to take a huge amount of atoms into account, which is only possible by the usage of interatomic potentials. Most known interatomic potentials are determined assuming that electrons are in their ground state and cannot describe nonthermal effects initiated by bond-softening or hardening. In order to take ultrafast thermal and non-thermal effects on the same theoretical level, Te-dependent interatomic potentials are needed. Here, we present an Te-dependent interatomic potential based, for the first time, on an artificial neural network. We studied silicon and show that the phonon band structure, the cohesive energy curves for several crystal structures, the electronic specific heat, atomic forces and cohesive energies are described in excellent agreement with DFT calculations for a wide range of Te. In addition, we simulated the laser-induced annealing of surface defects on a thin silicon film.

O 6.7 Mon 12:00 GER 39

Real-time TD-DFTB full periodic implementation for solids and low-dimensional materials — •Carlos R. Lien-Medrano[1], Franco P. Bonafé[2], Cristián G. Sánchez[3], and Thomas Fraeunheim[1] — [1]University of Bremen, Bremen, Germany — [2]MPSD, Hamburg, Germany — [3]University of Cuyo, Mendoza, Argentina

The current implementation of the real-time TD-DFTB dynamics for molecules and finite systems in the DFTB+ package[1] is based on the length gauge of the electric field. Here we show a proof-of-concept implementation of the vector potential in the velocity gauge of the electric field that in principle would allow us to extend the real-time dynamics to any periodic direction, making the new implementation suitable for the study of photo-induced dynamics processes in bulk, low-dimensional materials and surfaces. Instead of the dipole moment, the observable of choice is the frequency dependent conductivity which can be obtained from the Fourier transform of the autocorrelation function of the electric current density averaged over a unit cell. The conductivity provides access to the dielectric constant of the system allowing the calculation of optical properties.

[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 6.8 Mon 12:15 GER 39

Structure discovery in AFM imaging of ice — •Fabio Priante[1], Ye Tian[2], Dong Guan[2], Chen Xu[1], Shuning Cai[1], Niko Oinonen[1], Peter Liljeroth[1], Ying Jiang[2], and Adam Foster[1,3] — [1]Department of Applied Physics, Aalto University, Helsinki FI-00076, Finland — [2]International Center for Quantum Materials, Peking University, Beijing, 100871, China — [3]WPI Nano Life Science Institute (WPI-Nano LSI), Kanazawa University

The interaction of water with surfaces is crucially important in a wide range of natural and technological settings. Using high-resolution AFM and STM, several studies have demonstrated the presence of water pentamers, hexamers, heptamers (and of their combinations) on a variety of metallic surfaces. However, in all these situations, the observed structures were completely flat, providing a relatively straightforward path to interpretation. To address more complex cases, while simultaneously alleviating the interpretation effort, we develop an automated workflow centered around a convolutional neural network (to extract atomic positions) and a neural network potential (to rapidly sort candidate structures with high accuracy). We test our workflow on several high-resolution AFM measurements of water clusters on Cu(111), whose understanding is challenging due to both their highly 3D configuration and to their large size. For each of them, we propose an underlying atomic structure, finally comparing the experimental images with simulated AFM from Density Functional Theory. These results provide new insights into the early phases of ice formation, which is a ubiquitous phenomenon ranging from biology to astrophysics.

O 6.9 Mon 12:30 GER 39

Designing Covalent Organic Frameworks Through Active Machine Learning — •Yuxuan Yao[1,2], Christian Kunkel[3], Karsten Reuter[3], and Harald Oberhofer[2] — [1]Chair for Theoretical Chemistry, Technische Universität München — [2]Chair for Theoretical Physics VII, University of Bayreuth — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft

Covalent organic frameworks (COFs) are a class of materials, that are formed by molecular building blocks (BBs) connected with covalent bonds. They have found application in many fields such as catalysis, or optoelectronics. It is well known that their design space is far too large to sample one by one because numerous available BBs. We modify an earlier active machine learning (AML) approach that explores the massive available BBs space through the use of surrogate models for charge injection and transport descriptors. In this method, the Gaussian Process Regression(GPR) and AML are combined to train the molecular space. This way we ensure that only promising molecules that are very different from already explored ones have their descriptors evaluated by Density Functional based Tight Binding (DFTB) calculations. Specifically, we modify molecular generation rules in order to produce three-fold rotationally symmetric candidates molecules for use in hexagonal COFs. In the future this approach can be generalized for any other symmetries, to potentially even allow for 3-dimensional network generation. We gauge the performance of our AML by evaluating the success ratio, which is the ratio of promising candidates to all generated molecules.

O 6.10 Mon 12:45 GER 39

Machine-learning-backed evolutionary search for $SrTiO_3(110)$ surface reconstructions — •Ralf Wanzenböck, Florian Buchner, Jesús Carrete, and Georg K. H. Madsen — Institute of Materials Chemistry, TU Wien, Vienna, Austria

To determine the atomic structure of surface reconstructions, structural models derived from domain knowledge and intuition have historically been essential. Evolutionary algorithms combined with density functional theory have proven to be powerful tools for such structure searches if one accepts the prohibitive cost that comes with a thorough exploration of a potential energy surface. We train a neural-network force field (NNFF) as a surrogate model to drive the exploration of the rich phase diagram of TiO_x overlayers on $SrTiO_3(110)$ utilizing the covariance matrix adaptation evolution strategy (CMA-ES). We verify the transferability of the NNFF by performing CMA-ES runs on $SrTiO_3(110)$ 3×1, 4×1 and 5×1 with a model trained solely on 4×1 data. With the speedup afforded by the surrogate model we were able to perform exhaustive sets of exploratory runs to identify known and new low-energy reconstructions and match different symmetries found in experimental data. [R. Wanzenböck et al., Digital Discovery, 2022, 1, 703-710.]

O 7: Spins on Surfaces at the Atomic Scale I

Time: Monday 10:30–13:00 Location: REC C 213

Topical Talk O 7.1 Mon 10:30 REC C 213

Superconductivity in atom-by-atom crafted quantum corrals — •Lucas Schneider[1], Khai That Ton[1], Ioannis Ioannidis[2,3], Jannis Neuhaus-Steinmetz[1], Thore Posske[2,3], Roland Wiesendanger[1], and Jens Wiebe[1] — [1]Department of Physics, University of Hamburg, D-20355 Hamburg, Germany — [2]I. Institute for Theoretical Physics, University of Hamburg, D-20355 Hamburg, Germany — [3]Centre for Ultrafast Imaging, Luruper Chaussee 149, D-22761 Hamburg, Germany

Gapless materials in electronic contact with superconductors acquire proximity-induced superconductivity in a region near the interface. Here, we investigate the most miniature example of this so-called proximity effect on only a single quantum level of a surface state confined in a quantum corral on a superconducting substrate, built atom-by-atom using a scanning tunneling microscope. Whenever an eigenmode of the corral is pitched close to the Fermi energy by adjusting the corral's size, a pair of particle-hole symmetric states is found to enter the superconductor's gap. By comparison to a resonant level model of a spin-degenerate localized state coupled to a superconducting bath, we identify the in-gap states as scattering resonances theoretically predicted 50 years ago by K. Machida and F. Shibata, which had so far eluded detection. We further show that the observed anticrossings of the in-gap states indicate proximity-induced pairing in the quantum corral's eigenmodes. In a final step, we study how individual magnetic adatoms interact with the corral's eigenmodes.

O 7.2 Mon 11:00 REC C 213

Tailoring Yu-Shiba-Rusinov bands in a Kagome lattice by molecular self-assembly — •Laetitia Farinacci, Gael Reecht, Nils Bogdanoff, Benjamin W. Heinrich, Felix von Oppen, and Katharina J. Franke — Freie Universitaet Berlin, Germany

Coupling of magnetic bound states in superconductors (so-called Yu-Shiba-Rusinov or YSR states) leads to fascinating phenomena; such as the formation of topological states. Bottom up approaches allow for a precise characterization of the coupling parameters, shedding light onto the formation of YSR bands and their properties. Most studies so far rely on atom manipulation, which is time demanding and typically limits the size of the systems to below a hundred sites.

Here, we show that self-assembly of Fe-porphine-chloride (FePCl) molecules on Pb(111) can be controlled by varying the sample temperature during and after molecular deposition. In particular, we show that we can obtain islands in which the FeP molecules arrange in a Kagome lattice or in its precursors. This way, we can, on the one hand, characterize the YSR hybridization with molecular precision and, on the other hand, study the long-range band formation across 2D islands.

O 7.3 Mon 11:15 REC C 213

Atom-by-Atom Study of Spin Lattices on a Superconducting Rashba Material — •Khai That Ton, Lucas Schneider, Jens Wiebe, and Roland Wiesendanger — Department of Physics - University of Hamburg, Hamburg, Germany

In the research field of topological superconductivity, Rashba-spin-orbit-coupling is believed to be a stabilizing parameter for topological phases, increasing the size of the topological gap.

One well-known category of materials with large spin-orbit coupling are Bismuth-based surface alloys, which have been extensively studied by surface-sensitive methods like angle-resolved photoemission and scanning tunneling spectrosopy [1,2,3,4]. However, studies of such materials proximitized by superconducting substrates are lacking so far. In this work, we grew Bismuth-based surface alloys on thin films proximitized by elementary superconducting substrates, adsorbed transition metal atoms, and then built dimers, chains and small two-dimensional lattices of these atoms via STM-tip based atom manipulation. We will present a scanning tunneling spectroscopy investigation of the low-energy electronic structure of these different spin lattices.

[1] C. R. Ast et al. Phys. Rev. Lett. 98, 186807 (2007).

[2] C. R. Ast et al., Phys. Rev. B 75, 201401(R) (2007).

[3] M. Steinbrecher et al., Phys. Rev. B 87, 245436 (2013).

[4] W. Jolie et al., ACS Nano 16, 4876*4883 (2022).

O 7.4 Mon 11:30 REC C 213

Symmetry-dependent coupling in Yu-Shiba-Rusinov dimers — •Lisa Rütten[1], Eva Liebhaber[1], Harald Schmid[1], Gaël Reecht[1], Kai Rossnagel[2,3], Felix von Oppen[1], and Katharina Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24118 Kiel, Germany — [3]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

Unpaired adatom spins on superconductors interact with the Cooper pairs of the substrate and cause Yu-Shiba-Rusinov (YSR) states inside the superconducting gap. These can be probed by scanning tunneling spectroscopy at the single-atom scale. On superconducting van der Waals materials, the YSR wave functions of magnetic impurities can extend over several nanometers. This provides a wide range of adatom spacings over which their interaction is sufficiently strong to be potentially observed as a splitting in the tunneling spectra. Additionally, the YSR wave functions inherit their symmetry from the substrate. Depending on the symmetry and spacing in YSR dimers, the spins may interact differently via RKKY and Dzyaloshinskii-Moriya interactions. This manifests in splittings and/or shifts of the YSR states.

Here, we manipulate Fe atoms on superconducting $2H$-NbSe$_2$ using the tip of a scanning tunneling microscope and build dimers with different symmetries. Depending on the orientation of the dimers with respect to the crystal symmetry of the substrate we find YSR hybridization but also more complex effects caused by spin interactions.

O 7.5 Mon 11:45 REC C 213

Magnetic impurity states proposed as thermometer for superconducting quasiparticle temperatures — •Ciprian Padurariu[1], Sujoy Karan[2], Haonan Huang[2], Björn Kubala[1,3], Christian R. Ast[2], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

The occupation of the quasiparticle continuum in a superconductor is of critical importance for the functionality of Josephson junction-based quantum devices. While significant progress has been made recently, the detection and trapping of quasiparticles remains a significant challenge. This talk will describe the design of a thermometer that detects the presence and effective temperature of superconducting quasiparticles. The device consists of a mK-STM functionalized with a single Yu-Shiba-Rusinov (YSR) state inside the gap. Transport between the tip and a clean superconducting substrate shows Zeeman-split peaks in the differential conductance associated to the YSR state [1]. The current is sensitive to quasiparticles above the gap. We show, based on a simple rate equation model, how the control of the magnetic field, as well as the voltage bias, allows the operation of the junction as a thermometer for the effective temperature of quasiparticles.

[1] W.-V. van Gerven Oei, *et al.*, "Magnetic impurities in spin-split superconductors", Phys. Rev. B **95**, 085115 (2017).

O 7.6 Mon 12:00 REC C 213

Magnetic phase diagram of a YSR-molecule — •Niels P.E. van Mullekom[1], Benjamin Verlhac[1], Werner M.J. van Weerdenburg[1], Hermann Osterhage[1], Manuel Steinbrecher[1], Katharina J. Franke[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University Nijmegen, the Netherlands — [2]Fachbereich Physik, Freie Universität Berlin, Germany.

Yu-Shiba-Rusinov (YSR) states arise from the exchange coupling between a local spin and a superconductor, and are strongly linked to Kondo screening. Understanding the interplay of this exchange interaction with other energy scales, as well as the role of higher spin degrees of freedom, requires magnetic field dependent characterization. To date, most studies of YSR states have been limited to bulk superconductors, which easily quench in the presence of modest magnetic fields.

Here, using high resolution milliKelvin scanning tunneling microscopy and spectroscopy, we characterize the magnetic phase diagram of a molecule on the surface of a thin film superconductor. We see nontrivial changes in the YSR excitations, that go beyond the trends that are expected in a spin 1/2 picture. We relate these changes to the various properties of the molecule, including the role of multiple channels and magnetic anisotropy. We additionally propose a model to understand the various changes in the excitation. These results provide an in-depth and detailed approach to understand the role of high spin systems in the presence of Kondo and YSR states.

O 7.7 Mon 12:15 REC C 213

Spin currents in helical molecular wires — •Richard Korytár[1], Jan van Ruitenbeek[2], and Ferdinand Evers[3] — [1]Univerzita Karlova, Prague, Czech Republic — [2]Leiden University — [3]University of Regensburg

Various spin-selective phenomena have been recently reported for helical molecular wires. The explanation of these phenomena is still lacking [1]. I will present a theoretical analysis of spin currents in non-magnetic molecular junctions. First, constraints based on time-reversal invariance will be summarized. Second, I will present results based on Landauer formalism and a simple model Hamiltonian. Possible experimental detection setups will be discussed.

[1] Evers et al., Adv. Mater. 2022, 34, 2106629

O 7.8 Mon 12:30 REC C 213

Controlling the Spin States of iron porphyrin on Au(111) — •Xiangzhi Meng[1], Jenny Möller[2], Masoud Mansouri[3,4], Daniel Sánchez-Portal[3,4], Aran Garcia-Lekue[3,5], Alexander Weismann[1], Chao Li[1], 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 — [4]Centro de Física de Materiales CSIC-UPV/EHU, 20018 Donostia-San Sebastián, Spain; — [5]Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Spin-flip excitations of FeTBrPP molecules on Au(111) are investigated with a low-temperature scanning tunnelling microscope under ultrahigh vacuum condition. The molecules show two distinct adsorption configurations that exhibit different magnetic anisotropy energies. Density functional theory calculations show that the different structures and excitation energies reflect unlike occupations of the Fe 3d levels. We demonstrate that the magnetic anisotropy energy can be well controlled by adjusting the adsorption site, the orientation, or the tip-molecule distance.

O 7.9 Mon 12:45 REC C 213

Mapping magnetism with a molecule — •Alex Fétida[1], Michelangelo Romeo[1], Olivier Bengone[1], Marie-Laure Bocquet[2], Nicolas Lorente[3], and Laurent Limot[1] — [1]Université de Strasbourg, CNRS, IPCMS, UMR 7504, 67000 Strasbourg, France — [2]PASTEUR, Ecole Normale Supérieure, PSL University, Sorbonnes Université, CNRS, 24 Rue Lhomond, 75005 Paris, France — [3]Centro de Fisica de Materiales (CFM MPC) CSIC-EHU, 20018 San Sebastián, Spain

The decoration of metal probe-tips by a molecule intentionally picked up from a surface has proven to be a powerful method to improve the measurement capabilities of a scanning tunneling microscope (STM). The success of this approach opens the prospect of introducing spin sensitivity through the tip functionalization by a magnetic molecule. We show here that a metallocene-terminated tip can probe surface magnetism through the inelastic component of the tunneling current, which provides an electrical access to the metallocene spin states. When the tip is 100 picometers away from point contact, the exchange interaction between the tip and a magnetic sample changes the metallocene spin states. This detection scheme can then be used to independently measure the sample exchange field and spin polarization with atomic-scale resolution with knowledge of spin orientation as we show on ultra-thin cobalt layers.

O 8: Ultrafast Electron Dynamics at Surface and Interfaces I

Time: Monday 10:30–12:45 Location: TRE Phy

O 8.1 Mon 10:30 TRE Phy

Coulomb-correlated few-electron states from a laser-driven Schottky emitter — •Rudolf Haindl[1,2], Armin Feist[1,2], Till Domröse[1,2], Marcel Möller[1,2], Sergey V. Yalunin[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen — [2]4th Physical Institute, University of Göttingen

Observing correlation phenomena for free electrons requires a highly confined emission source, readily available by femtosecond photoemission from nanotips [1,2], and can in principle be studied using the supreme beam control provided by electron microscopes [3]. However, ensemble-averaged detection usually prevents studying multi-particle correlations in free-electron beams.

In this work, we use event-based electron microscopy to characterize laser-triggered few-electron pulses generated at a Schottky field emitter [4]. We find surprisingly strong energy correlations of about 2 eV in the two- and three-electron states hinting at a correlated emission process. Furthermore, state-sorted beam caustics show characteristic transverse pair distributions, as well as an increase and a longitudinal shift of the source.

Inducing strong few-electron Coulomb correlations facilitates non-Poissonian electron pulse statistics, promising applications in free-electron quantum optics.

[1] P. Hommelhoff, et al., Phys. Rev. Lett. 96, 077401 (2006).
[2] C. Ropers, et al., Phys. Rev. Lett. 98, 043907 (2007).
[3] A. Feist, et al., Ultramicroscopy 176, 63-73 (2017).
[4] R. Haindl, et al., arXiv:2209.12300 (2022).

O 8.2 Mon 10:45 TRE Phy

Impact of layer thickness on the anisotropic carrier dynamics of a laser-excited $\mathbf{Fe}_n/(\mathbf{MgO})_m(001)$ heterostructure from real-time TDDFT — •Elaheh Shomali, Markus Ernst Gruner, and Rossitza Pentcheva — Department of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen, Germany

The carrier dynamics of $\mathrm{Fe}_n/(\mathrm{MgO})_m(001)$ metal/insulator heterostructures has been investigated from first-principles as a function of the Fe and MgO layer thickness (n=1,3,5 and m=3,5,7), excitation energy and polarization direction. The imaginary part of the dielectric tensor calculated within the random phase approximation (RPA) shows for all structures a similar metallic-like behavior in the in-plane component, $\epsilon_{xx}(\omega)$, whereas for $\epsilon_{zz}(\omega)$ the initially low response below the MgO band gap for $\mathrm{Fe}_1/(\mathrm{MgO})_3(001)$ increases substantially with the number of Fe layers. Electronic excitations calculated in the framework of RT-TDDFT confirm the concerted excitation mechanism previously proposed for $\mathrm{Fe}_1/(\mathrm{MgO})_3(001)$ also for the larger systems, which involves two simultaneous excitations via interface states [1]: one from occupied states of the metal to the conduction band of the insulator and simultaneously, another from the valence band of MgO into Fe states above the Fermi level. This mechanism allows for an effective bidirectional relocation of excitations between the metallic and insulating subsystems even for photon energies below the MgO gap. Funding by DFG via SFB 1242, project C02 is gratefully acknowledged. [1] E. Shomali, M. E. Gruner, and R. Pentcheva, Phys. Rev. B **105**, 245103 (2022).

O 8.3 Mon 11:00 TRE Phy

Relaxation and transport dynamics of laser-excited electrons — •Markus Heckschen[1], Yasin Beyazit[1], Florian Kühne[1], Elaheh Shomali[1], Markus Gruner[1], Rossitza Pentcheva[1], Ping Zhou[1], Detlef Diesing[2], Axel Lorke[1], Uwe Bovensiepen[1], and Björn Sothmann[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [2]Faculty of Chemistry, University of Duisburg-Essen, Universitätsstraße 5, 45141 Essen, Germany

Scattering of electronic excitations after laser excitation is of key importance to understand transport and relaxation effects. A recent back-pump front-probe two-photon-photoemission experiment in Fe/Au samples measured the electron distribution as a function time and energy [1]. The time at which the maxima of the electron distribution occur as a function of Au-layer thickness provides information on velocity, transport regime and relaxation processes. Here, we present a trajectory-based simulation approach to describe the energy relaxation and the transport through the sample in the ballistic regime. Our results agree qualitatively with the experiment and provide new insight into ultrafast electron dynamics.

[1] Beyazit et al., PRL **125**, 076803(2020)

O 8.4 Mon 11:15 TRE Phy

Capturing non-thermal electrons: To what extend can a temperature-based model compete with a kinetic description? — •Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU, Kaiserslautern, Germany

The development and usage of laser systems in research allows to study the dynamics of laser-excited electrons in metals on sub-picosecond timescales. Kinetic models can trace non-equilibrium distributions in great detail for instance by using full Boltzmann collision integrals [1]. Due to the excitation of non-thermal electrons, this dynamics cannot be described with purely temperature-based models. However, there are a number of extensions of the well known two-temperature model to trace the non-thermal electrons in a numerically simplified way.

We aim to clarify, whether an extended TTM (first published in Refs. [2, 3], improved in Ref. [4]) can describe this electronic non-equilibrium dynamics by comparing it to the kinetic description. In particular, we compare the spectral particle dynamics to a time-resolved two-photon photoemission measurement [5].

[1] B. Y. Mueller and B. Rethfeld; Phys. Rev. B **87**, 035139 (2013)
[2] E. Carpene; Phys. Rev. B **74**, 024301 (2006)
[3] G. D. Tsibidis; Appl. Phys. A **124**, 311 (2018)
[4] M. Uehlein, S. T. Weber and B. Rethfeld;
Nanomaterials **12**, 1655 (2022)
[5] Y. Beyazit *et al.*; Phys. Rev. Lett. **125**, 076803 (2020)

O 8.5 Mon 11:30 TRE Phy

Radio-frequency controlled electron pulses for time-resolved LEED — •Dennis Epp[1], Benjamin Schröder[1], Marcel Möller[1], and Claus Ropers[1,2] — [1]Max-Planck-Institut für Multidisziplinäre Naturwissenschaften — [2]Georg-August-Universität Göttingen

In this contribution, we demonstrate temporal compression of low-energy electron pulses using rf-fields. Specifically, we combine a millimetre-sized electron gun [1] with a rf-cavity driven by a sinusoidal wave. A phase-locked loop synthesizer controls the timing between the incident electron pulses and the sinusoidal signal. By electron energy filtering, we measured an initial energy spread of ΔE*1.5 eV for the uncompressed pulses with mean kinetic energies in the range of 50 eV to 100 eV [2]. In perspective, ULEED with sub-ps resolution will allow for the observation of the impact of electron-phonon coupling and coherent vibrational motion on the efficiencies of surface phase transitions and the resulting changes in materials functionality. [1] Vogelgesang, et al., Nature Physics 14,184-190 (2018). [2] Epp et al., in preparation

O 8.6 Mon 11:45 TRE Phy

High-harmonic generation in topological insulator surface states using wave-packet approaches — •Vanessa Junk[1], Wolfgang Hogger[1], Alexander Riedel[1], Cosimo Gorini[2], and Klaus Richter[1] — [1]Institute for theoretical physics, University of Regensburg, Germany — [2]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

The interaction of matter with strong-field light gives rise to highly non-linear electron dynamics within the material. The electric field of the light accelerates electrons through the band structure and drives non-perturbative transitions, leading to strongly anharmonic electron velocities and the emission of high-order harmonics.

Here, we want to study these electron dynamics for the surface states of topological insulators by solving the time-dependent Schrödinger equation for wave packets. That the separation of bulk and surface high harmonics is experimentally possible has been demonstrated recently [1]. Furthermore, an alternating polarization rotation between odd and even order harmonics was found and attributed to the hexagonal warping present in Bi_2Te_3 surface states. Using effective Dirac models and taking into account effects of the Fermi sea, we can reproduce these experimental features with our wave-packet approach.

[1] C. Schmid, L. Weigl, P. Grössing, V. Junk, C. Gorini, S. Schlauderer, S. Ito, M. Meierhofer, N. Hofmann, D. Afanasiev, J. Crewse, K. Kokh, O. Tereshchenko, J. Güdde, F. Evers, J. Wilhelm, K. Richter, U. Höfer and R. Huber, Tunable non-integer high-harmonic generation in a topological insulator, Nature **593**, 385-390 (2021)

O 8.7 Mon 12:00 TRE Phy

Subcycle surface-bulk coupling in a topological insulator — •Suguru Ito[1], Michael Schüler[2], Manuel Meierhofer[3], Josef Freudenstein[3], Dmytro Afanasiev[3], Jens Güdde[1], Michael Sentef[4], Rupert Huber[3], and Ulrich Höfer[1] — [1]Philipps-Universität Marburg, Germany — [2]Paul Scherrer Institute, Switzerland — [3]Universität Regensburg, Germany — [4]Max Planck Institute for the Structure and Dynamics of Matter, Germany

Intense lightwaves at terahertz frequencies can drive currents in electronic bands as well as non-perturbative excitations across the band gap, whose interplay leads to strong-field phenomena such as high-harmonic generation. Angle-resolved photoemission spectroscopy (ARPES) with subcycle time resolution allows us to observe such lightwave-driven processes in momentum space.

Here, we will present our investigation of subcycle coupling between the topological surface state (TSS) and the bulk conduction band (BCB) in Bi_2Te_3, where the TSS is well seperated from the bulk along the $\bar{\Gamma}$-$\bar{\mathrm{K}}$ direction. Under exposure of a strong 25-THz lightwave, however, transient replicas of the equilibrium TSS, Floquet-Bloch states, are formed. Their hybridization with the BCB enables an efficient population transfer into the BCB. In contrast, TSS and BCB are less separated along $\bar{\Gamma}$-$\bar{\mathrm{M}}$, where already an intraband current can induce an efficient subcycle population transfer. Both distinct mechanisms are readily seen in our experiment. The dynamical Floquet-bulk coupling is confirmed by our full quantum calculations and provides a momentum-resolved view of non-perturbative interband excitations.

O 8.8 Mon 12:15 TRE Phy

Ultrafast electron dynamics in a topological crystalline insulator — •Magnus Berntsen[1], Yuzhu Fan[1], Antonija Grubisic-Cabo[1,2], Maciej Dendzik[1], Qinda Guo[1], Cong Li[1], Yang Wang[1], Wanyu Chen[1], Dibya Phuyal[1], Jonas Weissenrieder[1], and Oscar Tjernberg[1] — [1]Department of Applied Physics, KTH Royal Institute of Technology, Sweden — [2]University of Groningen, Netherlands

Topological crystalline insulators is a class of materials that possesses helical Dirac-like electronic surface states whose existence is protected by crystal symmetries. This intricate coupling of topology and crystal structure makes it particularly interesting to study the transient electronic structure in these materials induced by an optical excitation since an accompanying symmetry-breaking lattice deformation could lead to a break-down of the topological phase on an ultrafast time scale. Here, we have studied the ultrafast electron dynamics in the archetypal topological crystalline insulator (Pb,Sn)Se by time- and angle-resolved photoemission spectroscopy. The electronic excitation occurs mainly along a preferential direction in momentum space determined by the polarization of the pump pulse and the excitation spectrum displays multiple time scales suggestive of the existence of multiple relaxation channels. Supported by time-resolved diffraction data acquired by ultrafast electron microscopy, we discuss our findings both in the light of the specific electronic structure of the surface states as well as the potential influence of lattice dynamics on the decay of the electronic excitation.

O 8.9 Mon 12:30 TRE Phy

Field-induced ultrafast modulation of Rashba coupling in ferroelectric α-GeTe(111) — Geoffroy Kremer[1,2], Julian Maklar[3], Laurent Nicolaï[4], •Chris W. Nicholson[1,3,5], Changming Yue[1], Caio Silva[3], Philipp Werner[1], J. Hugo Dil[6,7], Juraj Krempaský[6], Gunther Springholz[8], Ralph Ernstorfer[3,9], Jan Minár[4], Laurenz Rettig[3], and Claude Monney[1] — [1]Université de Fribourg, Switzerland — [2]Université de Lorraine, France — [3]Fritz Haber Institute of the Max Planck Society, Germany — [4]University of West Bohemia, Czech Republic — [5]SPECS Surface Nano Analysis GmbH, Germany — [6]Paul Scherrer Institut, Switzerland — [7]EPFL, Lausanne, Switzerland — [8]Johannes Kepler Universität, Austria — [9]Technische Universität Berlin, Germany

Rashba materials provide an ideal playground for spin-to-charge conversion in prototype devices. I will present our recent time- and angle-resolved photoemission spectroscopy and momentum microscopy results on α-GeTe(111). This is a non-centrosymmetric ferroelectric (FE) semiconductor displaying a giant FE distortion below 700 K, which hosts spin-polarized states that are promising for a new type of highly efficient non-volatile memory device based on switchable polarization. We find a transient modification of the bulk Rashba splitting corresponding to an enhancement of the FE lattice distortion. This enhanced response results from a transient surface photovoltage which induces a delayed displacive excitation of a phonon along the FE distortion direction [1].

[1] Kremer et al, *Nature Communications* 13, 6396 (2022)

O 9: Focus Session: Frontiers of Electronic-Structure Theory I (joint session O/HL)

Electronic-structure calculations, based on density-functional theory (DFT) and methodology beyond, are getting increasingly involved as they face the following challenges: First, investigations of modern materials typically require large unit cells, owing to complex crystal structures, mixed compositions, internal interfaces, etc. Second, at the same time, they often require advanced methods, including hybrid functionals of DFT, Green-function techniques from many-body perturbation theory (MBPT), high-level wavefunction-based methods like coupled-cluster (CC) theory, or quantum Monte-Carlo simulations. All these methods should ideally be implemented in scientific software that is running efficiently on modern supercomputers. With both methodology and computer architectures exhibiting increasing complexity, collaborative development and shared tools, including ready-to-use libraries and codes, are becoming indispensable. This interdisciplinary symposium covers recent progress in the broad area of electron-structure methods and highly-sophisticated tools that enable the entire community to explore most exciting materials from different perspectives to either predict peculiar features or get insight into measured counterparts.

Organizers: Claudia Draxl (HU Berlin), Dorothea Golze (TU Dresden), Xavier Gonze (U Louvain), and Andris Gulans (U Latvia)

Time: Monday 10:30–13:00 Location: TRE Ma

O 9.1 Mon 10:30 TRE Ma

Testing the hell out of DFT codes with virtual oxides — Emanuele Bosoni[1], •Stefaan Cottenier[2], and Giovanni Pizzi[3] — [1]ICMAB-CSIC, Spain — [2]Ghent University, Belgium — [3]EPFL, Switzerland

If you use DFT to predict a property of a crystal, how confident can you be that the prediction is computed in a bug-free way? And if your DFT-code uses pseudopotentials, can you trust that the pseudopotential does not modify your predictions? Answering such questions has been the goal of a study a few years ago, in which 71 unary crystals were examined in exactly the same way by 40 different DFT methods and codes [DOI 10.1126/science.aad3000]. In a next step, a consortium of 41 scientists (*) has done a similar exercise for a much larger pool of crystals: all elements of the periodic table up to Z=96, each in 10 different crystal structures, 6 of them being (virtual) oxides that sample a range of chemical bond types and 4 being unary crystals that sample low to high coordination environments. In this presentation, we will discuss the reasons to choose these crystals, the different quality criteria by which results can be compared, we will demonstrate how this exercise leads to more precise and more trustworthy pseudopotential libraries, and we will show how this data set is shared with the community in order to foster better-tested codes and pseudopotentials for all.

(*) Unfortunately the size of this abstract does not allow to mention them all.

O 9.2 Mon 10:45 TRE Ma

High-throughput absorption spectra obtained by beyond-DFT workflows — •Fabian Peschel, Alexander Buccheri, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Fully converging *ab initio* calculations can be a challenging task, in particular when it comes to excited states, which require multiple ground-state calculations for different physical quantities. In this work, we aim at computing highly precise absorption spectra by employing the Bethe-Salpeter equation of many-body perturbation theory, as implemented in the all-electron full-potential package `exciting` [1,2]. To obtain benchmark data for a wide range of material classes, we have developed workflows where Python tools automatically create input files, start calculations, and evaluate results. For each material, all relevant input parameters, such as the number of k-points for the Brillouin-zone sampling, basis-set basis cutoff and the number of unoccupied states, are varied until the targeted convergence criteria are reached. With the help of a workflow manager, the calculations can be executed in a high-throughput fashion on a high-performance computing cluster. We demonstrate our approach with core-level spectra of elemental and binary solids, and provide an in-depth analysis of the obtained data. This work is carried out in the framework of the NOMAD Center of Excellence [3] and the CRC FONDA [4].

[1] A. Gulans et al., J. Phys. Condens. Matter **26**, 363202 (2014). [2] C. Vorwerk, B. Aurich, C. Cocchi, and C. Draxl, Electron. Struct. **1**, 037001 (2019). [3] https://nomad-coe.eu [4] https://fonda.hu-berlin.de

Topical Talk O 9.3 Mon 11:00 TRE Ma

Large-scale machine-learning assisted discovery and characterization of materials — •Miguel Alexandre Lopes Marques — Institut für Physik Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

In this talk we discuss our recent attempts to discover, characterize, and understand inorganic compounds using ab initio approaches accelerated by machine learning. We start by motivating why the search for new materials is nowadays one of the most pressing technological problems. Then we summarize our recent work in using crystal-graph attention neural networks for the prediction of materials properties. To train these networks, we curated a dataset of over 2 million density-functional calculations with consistent calculation parameters. Combining the data and the newly developed networks we have already scanned more than two thousand prototypes spanning a space of more than one billion materials and identified tens of thousands of theoretically stable compounds. We then discuss how simple, interpretable machine learning approaches can be used to understand complex material properties, such as the transition temperature of superconductors. Finally, we speculate which role machine learning will have in the future of materials science.

15 min. break

O 9.4 Mon 11:45 TRE Ma

Predicting the electronic structure at any length scale with machine learning — •Attila Cangi — Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany

The properties of electrons in matter are of fundamental importance. They give rise to virtually all molecular and material properties and determine the physics at play in objects ranging from semiconductor devices to the interior of giant gas planets. Calculations rely primarily on density functional theory (DFT), which has become the principal method for predicting the electronic structure of matter. While DFT calculations have proven to be very useful, their computational scaling limits them to small systems. We have developed a scalable machine learning framework for predicting the electronic structure on any length scale [1,2,3]. It shows up to three orders of magnitude speedup on systems where DFT is tractable and, more importantly, enables predictions on scales where DFT calculations are infeasible. Our work demonstrates how machine learning circumvents a long-standing computational bottleneck and advances science to frontiers intractable with any current solutions.

[1] J. A. Ellis, L. Fiedler, G. A. Popoola, N. A. Modine, J. A. Stephens, A. P. Thompson, A. Cangi, S. Rajamanickam, Phys. Rev. B 104, 035120 (2021). [2] L. Fiedler, N. Hoffmann, P. Mohammed, G. A. Popoola, T. Yovell, V. Oles, J. A. Ellis, S. Rajamanickam, A. Cangi, Mach. Learn.: Sci. Technol. 3 045008 (2022). [3] L. Fiedler, N. A. Modine, S. Schmerler, D. J. Vogel, G. A. Popoola, A. P. Thompson, S. Rajamanickam, A. Cangi, arXiv:2210.11343 (2022).

O 9.5 Mon 12:00 TRE Ma

Demonstrating temperature transferability of neural network models replacing modern density functional theory — •Lenz Fiedler and Attila Cangi — Helmholtz-Zentrum Dresden-Rossendorf / CASUS

Due to its balance between accuracy and computational cost, Density Functional Theory (DFT) is one of the most important computational methods within materials science and chemistry. However, current research efforts such as the modeling of matter under extreme conditions demand the application of DFT to larger length scales as well as higher temperatures. Such investigations are currently prohibited due to the computational scaling of DFT.

We have recently introduced a machine-learning workflow that replaces modern DFT calculations [1,2,3]. This workflow uses neural networks to predict the electronic structure locally. We show that by employing such an approach, models can be trained to predict the electronic structure of matter across temperature ranges. This paves the way for large-scale simulations of thermodynamically sampled observables relevant to modeling technologically important phenomena such as radiation damage in fusion reactor walls.

[1] J. A. Ellis *et. al*, Phys. Rev. B **104**, 035120

[2] L. Fiedler *et. al*, Mach. Learn.: Sci. Technol., **3** 045008

[3] L. Fiedler *et. al*, arXiv:2210.11343

O 9.6 Mon 12:15 TRE Ma

Pure non-local machine-learned density functional theory for electron correlation — •Johannes T. Margraf — Fritz-Haber-Institut der MPG, Berlin, Germany

Density-functional theory (DFT) is a rigorous and (in principle) exact framework for the description of the ground state properties of atoms, molecules and solids based on their electron density. While computationally efficient density-functional approximations (DFAs) have become essential tools in computational chemistry, their (semi-)local treatment of electron correlation has a number of well-known pathologies, e.g. related to electron self-interaction. Here, we present a type of machine-learning (ML) based DFA (termed Kernel Density Functional Approximation, KDFA) that is pure, non-local and transferable, and can be efficiently trained with fully quantitative reference methods. The functionals retain the mean-field computational cost of common DFAs and are shown to be applicable to non-covalent, ionic and covalent interactions, as well as across different system sizes.

O 9.7 Mon 12:30 TRE Ma

Predicting the response of the electron density to electric field using machine learning — •Alan Lewis and Mariana Rossi — MPI for Structure and Dynamics of Materials, Hamburg, Germany

The response of the electron density of a molecule or material to a homogeneous electric field defines its dielectric constant, along with its Raman and sum-frequency spectrum. We present a local and transferable machine learning approach capable of predicting the density response of molecules and periodic system on the same footing. This uses a very similar framework to that of the SALTED method recently introduced by these authors,[1,2] requiring only a small modification to the λ−SOAP descriptors used to represent the atomic environments. This allows us to predict the density response of liquid water to a field applied in each Cartesian direction from a single machine learning model. The tensorial dielectric constant can then be derived from this predicted density response, dramatically reducing the computational cost of calculating these properties relative to the standard approach of using density functional perturbation theory. We discuss the transferability of the model to different phases, and demonstrate the extrapolative power of this approach.

[1] Lewis, Grisafi, Ceriotti, Rossi, JCTC 17, 11, 7203 (2021)

[2] Grisafi, Lewis, Rossi, Ceriotti, accepted JCTC (2022)

O 9.8 Mon 12:45 TRE Ma

Analysis of Batching Methods in Graph Neural Network Models for Materials Science — •Daniel Speckhard, Tim Bechtel, Jonathan Godwin, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Berlin, Germany

Graph neural network (GNN) based models have shown promising results for materials science [1]. These models often contain millions of parameters, and like other big-data based models, require only a portion of the entire training dataset to be fed as a mini-batch to update model parameters. The effect of batching on the computational requirements of training and model performance has been thoroughly explored for neural networks [2] but not yet for GNNs. We explore two different types of mini-batching methods for graph based models, static batching and dynamic batching. We use the Jraph library built on JAX to perform our experiments where we compare the two batching processes for two data-sets, the QM9 dataset of small molecules and the AFLOW materials database [3]. We show that dynamic batching offers significant improvements in terms of computational requirements for training. We also present results on the effect of the batch size and batching method on model performance.

[1] T. Xie *et al.*, Physical Review Letters, 120, 14 (2018).

[2] M. Li *et al.*, Proceedings of the 20th ACM SIGKDD (2014).

[3] S. Curtarolo *et al.*, Comp. Mat. Science, 58, 227-235 (2012).

O 10: Organic Molecules on Inorganic Substrates II: Electronic, Optical and Other Properties II

Time: Monday 15:00–17:30 Location: CHE 89

Topical Talk O 10.1 Mon 15:00 CHE 89

Photoemission Orbital Tomography: Imaging Molecular Wave Functions in Reciprocal and Real Space — •F. S. Tautz — Quantum Nanoscience, Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany

The photoemission orbital tomography (POT) technique, a variant of angle-resolved photoemission spectroscopy, has been very useful in the characterization of the electronic properties of molecular films. It is a combined experimental and theoretical approach that is based on the interpretation of the photoelectron angular distribution in terms of a one-electron initial state. This includes the unambiguous assignment of emissions to specific molecular orbitals, their reconstruction to real space orbitals in two and three dimensions, the deconvolution of complex spectra into individual orbital contributions beyond the limits of energy resolution, the extraction of detailed geometric information such as molecular orientations, twists and bends, the precise description of the charge balance and transfer at interface, and the detection of momentum-selective hybridization with the substrate, to name only a few examples. In its simplest form, POT relies on the plane-wave approximation for the final state. While this works surprisingly well in many cases, this approximation does have its limitations, most notably for small molecules and with respect to the photon-energy dependence of the photoemission intensity. Regarding the latter, a straightforward extension of the plane wave final state leads to a much-improved description while preserving the simple and intuitive connection between the photoelectron distribution and the initial state.

O 10.2 Mon 15:30 CHE 89

Structural Reorientation of Organic Molecules on Surfaces by Alkali Metal Doping — •Ralf Hemm[1], Ka-Man Yu[1], Steffen-Rambert Rothenberg[1], Sergey Soubatch[2], Christian Kumpf[2], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,3] — [1]RPTU Kaiserslautern-Landau, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Johannes-Gutenberg-Universität Mainz, Staudingerweg 7, 55128 Mainz, Germany

Organic semiconductors are promising materials for the fabrication of next-generation organic-based electronic devices. The electron properties of the organic thin film can be tuned by alkali metal doping and the consequent charge transfer. Here, we study the influence of Cs doping on the structural and electronic properties of the model system PTCDA/Ag(111). Using momentum microscopy, we can simultaneously access changes in occupation of the molecular orbitals and determine modifications of the azimuthal orientation of the PTCDA molecules upon Cs doping. We can identify two structural Cs-PTCDA phases depending on the Cs concentration with either one or two Cs atoms per PTCDA. With increasing Cs concentration, we observe a gradual structural reorientation of the molecules that is accompanied by a modification of the population of the molecular states. Both cases are different from the pristine case. The structural reorientation of the PTCDA molecules can be attributed to the electrostatic interactions between the partially ionized Cs atoms and the negatively polarized oxygen end groups of PTCDA.

O 10.3 Mon 15:45 CHE 89

Tip-enhanced Raman Spectroscopy of a charged molecule — •Rodrigo Cezar de Campos Ferreira[1], Jiří Doležal[1,2], Amandeep Sagwal[1,2], Sofia Canola[1], and Martin Švec[1,3] — [1]Institute of Physics,Czech Academy of Sciences; Czech Republic — [2]Faculty of Mathematics and Physics, Charles University; Czech Republic — [3]Institute of Organic and Inorganic Chemistry, Czech Academy of Sciences; Czech Republic

The Tip-enhanced Raman spectroscopy (TERS) technique has been proven to unveil fundamental features of single molecules at the nanoscale level via near-field spectroscopy [1,2]. The confined light in the STM junction can be used as a probe to obtain an essential understanding of molecular structure and electronic properties. Here, the LT-STM-controlled TERS technique was performed and verified for the perylene tetracarboxylic dianhydride (PTCDA), which was measured the Raman fingerprint for a single molecule on Ag(111) and on insulating NaCl/Ag(111) from different excitation sources. Moreover, the precise control of geometry and charge state of the molecule in the system [3] can be observed together with the Raman fingerprint and revealed an abrupt change in the spectra. We correlate them to the presence of Kondo signature and discuss the implication for other systems.

[1] R. Zhang et al., Nature. 2013, 498, 82-86 [2] J.Lee et al., Nature. 2019, 568, 78-82 [4] M. Žonda et al., J.Phys.Chem.Lett. 2021, 12, 6320

O 10.4 Mon 16:00 CHE 89

Charge-induced symmetry breaking in the adsorption configuration of C60 layers on h-BN/Ni(111) — •Max Bommert, Roland Widmer, Néstor Diez, Bruno Schuler, and Oliver Gröning — Empa * Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

Hexagonal Boron Nitride (h-BN) and Nickel's (111) surface share a nearly perfectly matching lattice constant. Consequently, monolayer h-BN can be grown commensurately on Ni(111) without exhibiting a Moiré superstructure like on many other h-BN/transition metal systems. Nevertheless, upon adsorption at room temperature and scanning tunneling microscopy (STM) imaging at 5K, we observe a complex, geometrically frustrated adsorption pattern for sub-monolayer C60 coverages. The fullerenes form large molecular islands with a distinct striped pattern that we can identify as C60 adsorbed in different orientations. We use scanning tunneling spectroscopy (STS) to resolve the lowest unoccupied molecular orbitals (LUMO) of the C60. Tip-induced manipulation of single molecules affects the LUMO energy of neighboring molecules. Based on our STS investigations, we propose a significant charge transfer from the substrate to specific C60 and the associated electrostatic repulsion to be a driving force in forming the stripe pattern. We rationalize the latter by Monte Carlo simulations of the C60 lattice, considering the various contributions to the intermolecular and molecule-substrate interactions. Our results deepen the understanding of molecular adsorption and charge transfer processes, which are crucial for developing organic-inorganic hybrid devices.

O 10.5 Mon 16:15 CHE 89

Nickel(II) Porphyrins versus Nickel(II) Corroles on Different Metal Surfaces: Oxidation-State Tuning of Nickel Tetrapyrrole Complexes — •Jan Herritsch[1], Jan-Niclas Luy[1,2], Ralf Tonner-Zech[1,2], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Wilhelm-Ostwald-Institut, Leipzig, Germany

Using the example of Ni tetrapyrrole complexes, we demonstrate how the oxidation state of the central atom and the molecule-substrate interaction can be influenced by a modification of the ligand. In particular, the effect of the ring size is addressed by comparing porphyrins with corroles. The latter represent a smaller macrocycle and provide a tighter coordination environment for the metal center. In addition, Ni(II) corroles have an unusual electronic structure with an unpaired electron located at the π-electron system of the ligand. Here, we focus on the interactions of Ni(II) porphyrins and corroles with different metal surfaces (Au(111), Ag(111), Cu(111)). Depending on the used substrate, the Ni(II) porphyrin is subject to an interfacial charge transfer resulting in the reduction of the Ni atom as was shown by XPS. However, due to its unique properties Ni(II) corroles exhibit a different behavior at the metal/organic interface. While the corrole's Ni(II) state remains unchanged even on the reactive Cu(111) surface, the ligand is subject to a charge transfer by accepting electron density from the substrate. This charge transfer could be traced with experimental valence spectra (UPS), which were evaluated with the help of quantum chemical calculations (DFT).

O 10.6 Mon 16:30 CHE 89

Electronic Properties of N-Heterotriangulene Derivatives adsorbed on Au(111) — •Jakob Steidel[1], Ina Michalsky[2], Milan Kivala[2], and Petra Tegeder[1] — [1]Institute of Physical Chemistry, Heidelberg University, Im Neuenheimer Feld 253, 69120 Heidelberg — [2]Institute of Organic Chemistry, Heidelberg University, Im Neuenheimer Feld 270, 69120 Heidelberg

A large number of opto-electronic devices based on organic compounds utilize donor-acceptor-systems (D-A-systems), for example as the emitting layer in organic light emitting diodes or for charge separation in organic photovoltaics. Triphenylamine and its derivatives are a class of donors in D-A-systems with a high potential for applications in devices.

Introducing an etheno-bridge in the planar triphenylamine derivative indolo[3,2,1-jk]carbazole (N-heterotriangulene-550, N-HTA-550) closes an antiaromatic ring with seven members in the resulting N-heterotriangulene-557 (N-HTA-557). This significantly changes the electronic structure while retaining the molecular geometry as well as the steric demands. By oxidation of N-HTA-557 and a subsequent condensation reaction with quinoxaline-2,3-diamine an intramolecular D-A-system is created.

In the present contribution we study the electronic properties of N-HTA-550 and its derivatives on a Au(111) surface using two-photon photoemission spectroscopy.

O 10.7 Mon 16:45 CHE 89

Influence of N-introduction in pentacene on the electronic structure — •Mohsen Ajdari[1], Marvin Hoffmann[2], Felix Landwehr[1], Olena Tverskoy[3], Uwe H. F. Bunz[3], Andreas Dreuw[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen — [3]Organisch-Chemisches Institut, Universität Heidelberg

Organic electron-transporting (n-channel) semiconductors such as N-heteropolycyclic aromatic compounds are of great interest for use in a variety of (opto)electronic applications.

In this study, vibrational and electronic high-resolution electron energy loss spectroscopy (HREELS) in combination with quantum-chemical calculations are utilized to investigate the influence of N-introduction on the adsorption geometry and electronic structure of two pentacene derivatives, namely 6,13-diazapentacene (DAP) and 6,7,12,13-tetraazapentacene (TAP) on Au(111).

Our findings indicate that in comparison to parent pentacene (PEN), introduction of nitrogen atoms in the aromatic backbone of its aza derivatives leads to a narrowing of the optical gap ($S_0 \rightarrow S_1$ transition) from 2.1 eV for PEN to 2.0 eV for DAP and to 1.6 eV for TAP as well as an increase in the first triplet state energy from 0.9 eV for PEN and DAP to 1.2 eV in TAP. Additionally, In the series PEN, DAP, and TAP, the α-band ($S_0 \rightarrow S_2$ transition) gains significantly in intensity due to individual effects of the introduced nitrogen atoms on the orbital energies.

O 10.8 Mon 17:00 CHE 89

Electrostatic design of the internal surfaces of porous organic materials — •Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Collective electrostatic effects are ubiquitous at surfaces and interfaces involving organic materials. [1] Thus, they, for example, allow tuning the electronic properties of interfaces employing monolayers of molecules with embedded dipoles [2]. This raises the question, whether controlled assemblies of dipoles couldn*t also be used to control the properties of the inner surfaces of porous structures. This question is addressed for the prototypical case of layered covalent organic frameworks that are stacked in a way that 1D channels are formed. Employing state-of-the-art quantum-mechanical simulations, it is shown that by changing the polarity of the functional groups covering the surfaces of these pores, the electrostatic energy in the pores can be changed by more than one eV in a comparably straightforward manner. As this energy crucially determines the interaction between the host material and adsorbates within the pores, the proposed strategy holds the promise of revolutionizing various fields of application of such materials, e.g., as battery electrodes, in catalysis, and in excited-state charge separation processes. [1] E. Zojer, T. C. Taucher, and O. T. Hofmann, Adv. Mater. Interf. (Hall of Fame Review), 1900581 (2019); [2] E. Zojer, A. Terfort, and M. Zharnikov, Acc. Chem. Res. 55, 1857 (2022)

O 10.9 Mon 17:15 CHE 89

Screening Non-alternant π-Electron Systems for Metal-Organic Interfaces: Interplay between Topology, Aromaticity, and Adsorption Behavior — •Jakob Schramm and Ralf Tonner-Zech — Universität Leipzig, Deutschland

Metal-organic interfaces play an important role in organic electronics. Topology, aromaticity, and interface properties are closely connected here as previously shown by experimental and theoretical studies of isomer pairs of alternant and non-alternant adsorbates. While non-alternant azulene and azupyrene chemisorb on Cu(111), the alternant isomers naphthalene and pyrene physisorb.[1,2] This promises to be a general trend and can be exploited for interface design.

Here, we report data based on periodic DFT calculations for a set of 11 non-alternant molecules in comparison to analogous alternant molecules. Influence of topology on atomic and electronic structure, especially aromaticity, was analyzed based on molecular gas phase calculations. Interface properties were then derived using slab approaches at the example of Cu(111). We report on the interplay of topology and adsorption structure, adsorption energy, and charge transfer.

[1] B. P. Klein, R. Maurer, R. Tonner, C. Kumpf, I. Swart, J. M. Gottfried et al., Phys. Rev. X. 2019, 9, 011030; [2] B. P. Klein, R. Maurer, G. Hilt, R. Tonner-Zech, A. Schirmeisen, J. M. Gottfried et al., ACS Nano 2022, 16, 11979-11987.

O 11: Surface Reactions

Time: Monday 15:00–17:15 Location: CHE 91

O 11.1 Mon 15:00 CHE 91

Machine-Learning Driven Global Optimization of Surface Adsorbate Geometries — •Hyunwook Jung, Lena Sauerland, Sina Stocker, Karsten Reuter, and Johannes T. Margraf — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The adsorption energies of molecular adsorbates on catalyst surfaces are key descriptors in computational catalysis research. For the relatively large reaction intermediates frequently encountered, e.g., in syngas conversion, a multitude of possible binding motifs leads to complex potential energy surfaces (PES), however. This implies that finding the optimal structure is a difficult global optimization problem, which leads to significant uncertainty about the stability of many intermediates. To tackle this issue, we present a global optimization protocol for surface adsorbate geometries which trains a surrogate machine learning potential on-the-fly. The approach is applicable to arbitrary surface models and adsorbates and minimizes both human intervention and the number of required DFT calculations by iteratively updating the training set with configurations explored by the algorithm. We demonstrate the efficiency of this approach for a diverse set of adsorbates on the Rh(111) and (211) surfaces.

O 11.2 Mon 15:15 CHE 91

The effect of ultrathin ionic liquid films on the adsorption dynamics of 1,3-butadiene and 1-butene on Pt(111) studied by molecular beam techniques — •Leonhard Winter, Cynthia Carolina Fernández, Afra Gezmis, Timo Talwar, Stephen Massicot, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Ionic Liquids (ILs) are low temperature melting salts. In “Solid Catalyst with Ionic Liquid Layer (SCILL)” systems, IL thin films are used to coat the catalytically active metal and thereby enhance the selectivity of the catalyst; this approach is beneficial, e.g., in the industrially important hydrogenation of 1,3-butadiene to butenes, since further hydrogenation to *n*-butane must be suppressed. We used a supersonic molecular beam to investigate the adsorption dynamics of this reaction in a UHV SCILL model system. Along the method of King and Wells we measured sticking coefficients of 1,3-butadiene and 1-butene on Pt(111) coated with ultrathin layers of the IL 1,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide ($[C_1C_1Im][Tf_2N]$). At 180 K, the sticking coefficients decrease non-linearly with increasing IL coverage. We explain the deviation from a simple site-blocking model with trapping into a mobile precursor state of the hydrocarbon molecules that arrive on top of IL islands. This deviation is less pronounced for films prepared at 250 K, which we attribute to larger IL island sizes.

Supported by the DFG through SFB 1452 CLINT.

O 11.3 Mon 15:30 CHE 91

On-surface synthesis of porphyrinoid monomers and dimers — •Hongxiang Xu[1], Ritam Chakraborty[2], Biao Yang[1], Joachim Reichert[1], Abhishek K. Adak[2], Shobhana Narasimhan[2], Johannes V. Barth[1], and Anthoula C. Papageorgiou[1,3] — [1]Technical University of Munich, Germany — [2]Jawaharlal Nehru Centre for Advanced Scientific Research, India — [3]National and Kapodistrian University of Athens, Greece

Porphyrinoid molecules can incorporate a wide array of the elements of the periodic table in a chemical pocket. By engineering their coordination pocket one can tune the functional properties for catalysis, spintronics, electronics and sensors. Here we use a common natural pigment, indigo, with Fe atoms on Au(111). By a series of thermally activated reaction steps including selective C-H activation, we obtain a novel metallated porphyrinoid species with high yield. By McMurry-type coupling on the same surface, this porphyrinoid species fuses into dimers. The reaction products are identified by a combination of scanning tunnelling microscopy, bond resolving atomic force microscopy and density functional theory investigations. Our studies expand the available chemistry for on-surface synthesis of macrocyclic tetrapyrroles [1] and contribute to versatile metal-organic nanostructures with smaller coordination pockets, which are challenging to obtain via solution chemistry.

[1] E. Nardi, et al. *J. Phys. Chem. C* 2014, **118**, 27549; Q. Fan, et al. *Nat. Commun.* 2019 **10**, 5049.

O 11.4 Mon 15:45 CHE 91

Fischer-Tropsch synthesis on magnetite (111) surface — •Heshmat Noei[1], Robert Gleissner[1], Michael Wagstaffe[1], Christopher Goodwin[2], Markus Soldemo[2], Mikhail Shipilin[2], Patrick Lömker[2], Christoph Schlueter[3], Peter Amann[2], and Andreas Stierle[1] — [1]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [2]Stockholm Universitet, Department of Physics, Roslagstullsbacken 21, 10691 Stockholm, Sweden — [3]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

Magnetite (Fe_3O_4) is an important and diverse transition metal oxide with applications in catalysis, data storage and biomedical imaging. In this contribution, we demonstrate an operando Fischer-Tropsch synthesis with a focus on product detection on the magnetite (111) surface and clarify the reaction mechanism and intermediates applying state of the art ambient pressure XPS with ability to measure photoemission spectra 76 at above 1 bar using hard X-ray at PETRA III beamline at DESY in Hamburg and clarify the mechanism of FT synthesis by monitoring reaction products operando on single crystal Fe_3O_4. We show then the dominant product from FT synthesis is a methoxy species and short chain alkanes under our reaction conditions (500 mbar, 400°C) and that no aldehydes and ketones are formed during reaction.

O 11.5 Mon 16:00 CHE 91

On-Surface CO_2 Capturing by Electron-Rich Phosphines: Comparison of the Assembly on Ag(100) and on the NaBr(100) Double Layer — •Vladimir Lykov[1], Florenz Buss[2], Fabian Dielmann[3], and Karina Morgenstern[1] — [1]Ruhr-Universität Bochum, Germany — [2]Institut für Anorganische und Analytische Chemie, Westfälische Wilhelms-Universität Münster, Ger-

many — [3]Institute of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Center for Chemistry and Biomedicine, Innsbruck, Austria

Electron-rich phosphines exhibit exceptional electron donor properties and form zwitterionic Lewis base adducts with small inert molecules, for instance, carbon dioxide (CO_2) and sulfur dioxide (SO_2) [1]. The main focus of this project is understanding the influence of geometrical confinement on the capturing of CO_2 by electron-rich phosphines. The effect of geometrical confinement is studied with a surface science approach. For this purpose, we use a low-temperature (7 K) scanning tunneling microscope (STM). To understand the influence of the metal surface on carbon dioxide capture, we compare the molecules adsorbed on Ag(100) to those on NaBr(100) double layer, supported by Ag(100). The subsequent deposition of carbon dioxide and electron-rich phosphines confirmed the affinity of CO_2 to these phosphines. The influence of the two surfaces on the product assembly will be discussed in this presentation.

[1] F. Buß, et al. Chem. Eur. J. 2022, 28, e2021040.

O 11.6 Mon 16:15 CHE 91

On-surface synthesis of enetriynes — Nan Cao[1,2], •Biao Yang[1], Alexander Riss[1], Johanna Rosen[2], Jonas Björk[2], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, Garching, Germany — [2]Department of Physics, Chemistry and Biology, IFM, Linköping University, Linköping, Sweden

Belonging to the enyne family, enetriynes comprise a distinct electron-rich all-carbon bonding scheme. However, the lack of convenient synthesis protocols limits the associated application potential within, e.g., biochemistry and materials science. Herein we introduce a pathway for highly selective enetriyne formation via tetramerization of terminal alkynes on a Ag(100) surface. Taking advantage of a directing hydroxyl group, we steer molecular assembly and reaction processes. Induced by O2 exposure the terminal alkyne moieties deprotonate and organometallic bis-acetylide dimer arrays evolve. Upon subsequent thermal annealing tetrameric enetriyne-bridged compounds are generated in high yield, readily self-assembling into regular networks. We combine high-resolution scanning probe microscopy, X-ray photoelectron spectroscopy and density functional theory calculations to examine the structural features, bonding characteristics and the underlying reaction mechanism. Our study provides an integrated strategy to precisely fabricated functional enetriyne species, providing access to a distinct class of highly conjugated π-system compounds.

O 11.7 Mon 16:30 CHE 91

Cold plasma deoxidation of copper and iron surfaces — •Viktor Udachin[1], Sebastian Dahle[2], and Wolfgang Maus-Friedrichs[1] — [1]Clausthal University of Technology, Clausthal-Zellerfeld, Germany — [2]University of Ljubljana, Ljubljana, Slovenia

The removal of native oxides, which are present on metals in ambient atmosphere, is an important step in many industrial applications. Cold plasma methods, like dielectric barrier discharge (DBD) plasmas, have gained attention due to the high deoxidation efficiencies and relative simplicity of the setups. Several groups have indicated a reduction of copper oxygen layers using DBD hydrogen-containing plasmas, but no detailed information about reduction kinetics and limitations on different metal systems is available. In this study, we investigated the deoxidation effect of a DBD plasma in Ar/H_2 and Ar/SiH_4 atmospheres on natively oxidized Cu and Fe surfaces at 1000 hPa. We observed deoxidation effect on Cu already at 25 °C in both atmospheres. In contrast, reduction of iron oxide was obtained only at the surface temperature of 200 °C, showing an increase in the efficiency of the plasma-induced thermal treatment in comparison to thermal one. The chemical state of the samples and the kinetics of the reduction of oxides were studied via X-ray photoelectron spectroscopy (XPS). The morphology was characterized with the atomic force microscopy (AFM). By using optical emission spectroscopy (OES), the reactive species within the implemented DBD plasmas were described.

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O 11.8 Mon 16:45 CHE 91

Multiscale modeling and simulation of texture effects on the corrosion of stainless steel in aqueous media — •Vahid Jamebozorgi[1,2], Karsten Rasim[3], and Christian Schröder[1,2] — [1]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences, 33619 Bielefeld, Germany — [2]Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [3]Miele & Cie. KG, Center for Materials (CFM), Carl-Miele-Straße 29, 33332 Gütersloh

Texture plays a crucial role in physical processes and properties of condensed matter as it is broadly highlighted in the literature. In this work we describe a robust methodology to investigate texture effects which does not suffer from common limitations of quantum based computational approaches in time and space but also can provide the same accuracy as atomistic calculations with orders of magnitude less computational costs. Our methodology is based on the finite element method (FEM) and utilizes 3D digital representations of multi grain microstructures. We demonstrate the efficiency of our approach by studying pitting corrosion in stainless steel. As reflected in literature the irregular geometry of pit expansion through pitting corrosion is mostly caused by texture. We found that the texture significantly affects the pitting corrosion rate and consequently causes various irregular pit growth patterns in granular microstructures. These results are consistent with our DFT and reactive force field molecular dynamics simulations which validates our suggested approach.

O 11.9 Mon 17:00 CHE 91

The role of aromaticity in the cyclization and polymerization of alkyne-substituted porphyrins on Au(111) — •Nan Cao[1], Jonas Björk[2], Eduardo Corral-Rascon[1], Zhi Chen[3,4], Mario Ruben[3], Mathias O. Senge[5], Johannes V. Barth[1], and Alexander Riss[1] — [1]Technical University of Munich, Germany — [2]Linköping University, Sweden — [3]Karlsruhe Institute of Technology, Germany — [4]Shenzhen University, China — [5]Institute for Advanced Study, TUM, Germany

Aromaticity is one of the most practical and versatile concepts for the assessment of the reactivity of organic molecules. However, in on-surface chemistry - where the interaction with the substrate can significantly alter the electronic and geometric structure of the adsorbates - the role of aromaticity is not understood. Here we investigate how aromaticity affects the reactivity of alkyne-substituted porphyrin molecules in cyclization and coupling reactions on a Au(111) surface.[1] We examine and quantify the regioselectivity of the reactions by scanning tunneling microscopy and bond-resolved atomic force microscopy at the single-molecule level. Our experiments show a substantially lower reactivity of carbon atoms that are stabilized by the aromatic diaza[18]annulene pathway of free-base porphyrins. The results are corroborated by density functional theory calculations, revealing a direct correlation between aromaticity and thermodynamic stability of the reaction products. These insights will help to design and understand reactions in on-surface chemistry and heterogeneous catalysis.
1. https://doi.org/10.21203/rs.3.rs-1271465/v1

O 12: Scanning Probe Techniques: Method Development I

Time: Monday 15:00–17:00 Location: GER 37

O 12.1 Mon 15:00 GER 37

Performance boundaries of piezoelectric friction-inertia walkers due to the choice of contact materials — ●Felix Huber, Susanne Baumann, and Sebastian Loth — University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany

High precision positioners are an important tool to realize and automate cutting edge experiments. Piezoelectric friction-inertia walkers enable high accuracy movement on the millimeter scale with nanometer resolution, which makes them essential to realize scanning probe microscopes. The working principle of these nanopositioners makes use of the friction-inertia principle [1]. Therefore, the choice of materials for the contact surfaces defines the performance limits and the reproducibility of stepwise motion. We use optical interferometry to determine the key performance parameters of a linear piezoelectric friction-inertia walker and test combinations of metallic and ceramic contact surface materials to improve the capabilities and reliability of high precision positioner devices.

[1] Z.M. Zhang et al. (2012) Int J Adv Manuf Technol 62, 669-685

O 12.2 Mon 15:15 GER 37

Surface tension measurement of microdroplets using AFM — ●Pranav Sudersan[1], Mohammad Hormozi[2], Maren Müller[1], Shuai Li[1], Hans-Jürgen Butt[1], and Michael Kappl[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Technical University of Darmstadt, Darmstadt, Germany

Surface tension is a physical property which is central to our understanding of wetting phenomena. One could easily measure liquid surface tension using commercially available tensiometers. However, these tensiometers are designed for bulk liquid volumes of the order of millilitres. In order to perform similar measurements on extremely small sample volumes in the range of femtoliters, Atomic Force Microscopy (AFM) is a promising tool. It was previously reported that by fabricating a special 'nanoneedle' shaped cantilever probe, a Wilhelmy-like experiment can be performed with an AFM. In our study, we carried out measurements on microscopic droplets with the AFM, but instead using standard pyramidal cantilever tips. The AFM tips were coated with a hydrophilic polymer brush, which reduced its contact angle hysteresis. Numerical simulations of a liquid drop interacting with a pyramidal geometry were used to calculate surface tension from the experimentally measured force. Our method eliminates the need for specially fabricated 'nanoneedle' tips, thus reducing complexity and cost of measurement, making it more suitable for widespread application.

O 12.3 Mon 15:30 GER 37

Modification of Fluid-FM Cantilevers for Studying Local Electrochemistry at Solid | Liquid Interfaces — ●Matin Karimnia[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 (KIT), Karlsruhe, Germany

Local electrochemical measurements at the solid | liquid interface are of particular interest to gain deeper insights into the structure-activity relationship for electrochemical systems. Atomic force microscopy (AFM), can be effectively used for *in situ* monitoring of electrochemical processes, including adsorption, and metal deposition[1−4]. For a better resolution of local phenomena, in this work, we present the use of Fluid-FM. Here the cantilever has a hollow microfluidic channel, allowing for probing electrochemical processes in the vicinity of the tip. This can be achieved by modifying the Fluid-FM cantilever to serve as a counter electrode in the electrochemical cell formed by the tip and the investigated substrate. The feasibility of the approach is demonstrated using a Au surface in contact with a diluted H_2SO_4 electrolyte. The influence of parameters such as the ratio between the surface area of the working electrode and counter electrode, as well as the volume of the electrolyte on the electrochemical performance is discussed.

[1] Seo, Yongho, *et al.* *Rep.Prog.Phys.* **71** (2007): 016101. [2] Oorschot, Ralph, *et al.* *Techn. Instrum.* **2** (2015): 1-11. [3] Zampardi, Giorgia, *et al.* *RSC Adv.* **5** (2015): 31166-31171. [4] Ossola, Dario, *et al.* *Phys. Rev. Let.* **115** (2015): 238103.

O 12.4 Mon 15:45 GER 37

Analysis of DNA-origami-based calibration standard for AFM using artificial intelligence — ●Ziba Akbarian[1,2], Tim Johannes Seifert[1], Birka Lalkens[2], Ingo Busch[3], Harald Bosse[3], and Uta Schlickum[1,2] — [1]Technische Universität Braunschweig, Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology (LENA), Braunschweig, Germany — [3]Physikalisch Technische Bundesanstalt, Braunschweig, Germany

In this investigation, we focus on a nanoscale-standard reference system for calibrating atomic force microscopes utilizing DNA origami. To introduce measurable protrusions on the DNA origami nanostructure, markers at well-defined positions have been attached. To analyze the nanostructures as accurately as possible, we propose the use of artificial intelligence (AI) based image analysis techniques. Commonly, evaluation of the obtained data from atomic force microscopes is performed manually and includes preparatory steps to visualize images before analysis. As a result, the data analysis process requires a lot of time and always introduces not-avoidable errors. We present an AI-based measurement procedure using the YOLOv5 object detection and a semantic segmentation network trained on synthetic data to crop origami structures and pixelwise locate markers, respectively. This way, we can achieve a relative calibration accuracy in the range of 1% with an automatic data evaluation tool.

O 12.5 Mon 16:00 GER 37

Interplay between magnetic and electrostatic forces when imaging complex current carrying stripline geometries with Magnetic Force Microscopy — Denis Goman, Dhavalkumar Mungpara, and ●Alexander Schwarz — Institute of Nanostructure and Solid State Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg

Current carrying strip-lines have been oftentimes used to calibrate the sensitivity of magnetic tips to perform quantitative magnetic force microscopy, because for this system the Oersted field can be calculated analytically. In these investigations possible electrostatic contribution to the measured signal have been usually ignored.

Our research focuses on more complex strip-line arrangements with meander and spiral geometries, which are part of a magnetometer. Current dependent magnetic force microscopy (MFM) images clearly show that the measured signal possesses a large electrostatic contribution, which, in a peculiar fashion, depends on the tip location. We find that electrostatic contributions stem from three sources: (i) the contact potential difference between strip-line and substrate material, (ii) the potential drop along the strip-line and (iii) an edge effect related to the finite size of the tip apex. This knowledge helps to disentangle magnetostatic and electrostatic contributions even for rather complex strip-line geometries.

This work has been conducted as part of the OXiNEMS project, which has received funding from the European Union's Horizon 2020 research and innovation program under Grant Agreement No. 828784.

O 12.6 Mon 16:15 GER 37

Influence of Surfaces Charges and Trap States in KPFM Measurements of Doping Concentration — ●Thilo Glatzel, Urs Gysin, and Ernst Meyer — University of Basel, Department of Physics, Klingelbergstr. 82, 4056 Basel, Switzerland

Kelvin Probe Force Microscopy is a scanning probe method for imaging the surface potential by atomic force microscopy. The surface potential is one of the most important surface properties and is correlated to e.g. the work function, surface dipoles, localized surface charges, and structural properties. It gives detailed information on the electrical properties and can be combined with optical and electrical excitation mechanisms providing additional properties like surface band bending and charge carrier mobilities. We will introduce the main concept and will briefly describe the major methods of operation. Based on the analysis of a Si super-junction device structures dopant profiling and the concept of surface photovoltage measurements will be introduced. The influence of local charge accumulation and trap states on these devices will be presented and the effect on the measured contact potential values will be discussed.

O 12.7 Mon 16:30 GER 37

Development of SNOM combining plasmonic picocavities with noncontact AFM — •Akitoshi Shiotari[1], Jun Nishida[2], Adnan Hammud[1], Martin Wolf[1], Takashi Kumagai[2], and Melanie Müller[1] — [1]Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]Institute for Molecular Science, Okazaki, Japan

Scattering-type scanning near-field optical microscopy (s-SNOM) is a powerful tool to visualize the nanoscale optical response of sample surfaces. However, the resolution of conventional s-SNOM is usually limited by thermal instabilities of the tip-apex structure and the weak light intensities scattered from small volumes. On the other hand, it has been shown recently that light can be confined to the atomic scale using plasmonic picocavities. Here we demonstrate the development of plasmonic s-SNOM based on noncontact atomic force microscopy (nc-AFM) under the low-temperature and ultrahigh-vacuum conditions. A quartz tuning fork sensor with a Ag tip sharpened by focused ion beam milling enables precise control of the subnanometer tip-sample gap under illumination with visible laser light. The extremely high field enhancement and localization of light in the picocavity enhances the scattered light intensity and allows to image the optical response of samples at 1 nm resolution. The combination of ncAFM with plasmonic picocavities has high potential for atomic resolution optical imaging of various materials, including insulators.

O 12.8 Mon 16:45 GER 37

Polarization-sensitive scanning near-field optical microscopy — •Felix G. Kaps[1,2], Susanne C. Kehr[1,2], and Lukas M. Eng[1,2] — [1]Technische Universität Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence - EXE 2147 (ct.qmat), Dresden, Germany

Scanning near-field optical microscopy (SNOM) enables nanoscopic optical surface characterization at visible, infrared, and THz wavelengths [1], with applications to various research fields e.g. 2D materials, semiconductors, and in biology [2]. Here, typically the pure out-of-plane field components are considered. For resonant samples however, near-field excitation of all vectorial components becomes possible [3], enabling the full polarization analysis at the nanometer length scale.

In the work presented here, we examine the polarization-dependent near-field response of both non-resonantly (Au) and resonantly (SiC) excited samples at around 10.6 μm. By varying the incident linear polarization direction from s- to p-polarization, we are able to capture differently scattered near-field contributions, showing up in characteristic lobe-shaped polarization signatures. These results are confirmed by theoretical simulations, where we combine the analytic dipole model [5] and the Jones matrix formalism. Comparing the experiment with our simulations, we are able to disentangle the near-field‘s vectorial contributions via spectral and polarization analysis.

[1] T. Nörenberg etal., *ACS Nano*, **article ASAP** (2022)
[2] T.V.A.G. de Olivera et al., *Adv. Mater.* **33**, 2005777 (2021).
[3] H. Aminpour et al., *Opt. Express* **28**, 32316 (2020)

O 13: Focus Session: Ion Beam Interaction with Surfaces and 2D Materials II

Time: Monday 15:00–17:15 Location: GER 38

Topical Talk O 13.1 Mon 15:00 GER 38

Space weathering of planetary surfaces — •Peter Wurz — Physics Institute, University of Bern, Bern, Switzerland

The surfaces of planetary objects in interplanetary space are subjected to external agents modifying their chemical and mineralogical composition and causing removal of material from these surfaces into interplanetary space. These external agents are the flow of ions and electrons from the Sun (the solar wind), currents of magnetospheric systems, energetic particles from outer space, impacting micro-meteorites, and photons from the Sun. In particular, the ion precipitation on these surfaces is of high interest. The removal of surface material, e.g., the ion-induced sputtering, contributes atoms to the interplanetary particle population, which eventually end up as ions in the interplanetary plasma flow. The changes in composition of the surface are also of interest because they affect the spectroscopic appearance of these surfaces. Since most of the planetary objects are only studied via telescopic observations, relating the spectroscopic appearance of the space-weathered surface to the underlying material is of high importance.

O 13.2 Mon 15:30 GER 38

Quantifying the erosion of the lunar surface due to solar wind sputtering — •Johannes Brötzner[1], Herbert Biber[1], Noah Jäggi[2], Paul Stefan Szabo[3], Daniel Primetzhofer[4], André Galli[2], Peter Wurz[2], and Friedrich Aumayr[1] — [1]TU Wien, Institute of Applied Physics, Vienna, Austria — [2]University of Bern, Physics Institute, Bern, Switzerland — [3]University of California, Space Sciences Laboratory, Berkeley, USA — [4]Uppsala University, Department of Physics and Astronomy, Uppsala, Sweden

Without a protective atmosphere nor its own magnetic field, the lunar surface is subjected to bombardment by the solar wind, a stream of mostly H^+ and He^{2+} ions originating from the Sun. Combined with other effects, this leads to the ejection of material and subsequently the formation of a tenuous gas layer around the Moon, the exosphere. Understanding its formation and coupling to surface properties could potentially enhance our knowledge of not only the Moon, but also other rocky bodies in the solar system.

Previous attempts at modelling the creation of an exosphere used sputter yield values of limited validity for the sputtering contribution to this process – data for relevant minerals were simply not available. While in the past few years, investigations using adequate analogue materials have progressed, we present both experimental and numerical results for the irradiation of H^+ and He^+ ions on samples prepared from actual lunar material, gathered during the Apollo 16 mission in 1972.

O 13.3 Mon 15:45 GER 38

Sputtering from Sinusoidal Surfaces: Monte Carlo Simulations and Comparison to Analytical Results — •Gerhard Hobler[1] and R Mark Bradley[2] — [1]Institute of Solid-State Electronics, TU Wien, AUSTRIA — [2]Departments of Physics and Mathematics, Colorado State University, Fort Collins, CO 80523, USA

Sputtered surfaces are virtually never planar at the nanoscale, and so there has been longstanding interest in the spatially averaged sputter yield $\bar{Y}$ that results when a broad ion beam is incident on a surface with a nontrivial morphology. Considering the simple case of sinusoidal surfaces, the aim of the present study is (i) to investigate the contributions of redeposition and secondary sputtering to $\bar{Y}$, and (ii) to test a recently developed theory [1] that predicts $\bar{Y}$ for small amplitudes from the angular dependent sputter yield of a flat surface. For the simulations we use the Monte Carlo binary collision code IMSIL [2]. Apart from expected results on redeposition and sputtering by reflected ions, we also find that sputtering by recoils that are sputtered and then strike the surface may compensate for a sizable amount of redeposition. The simulations confirm the theory's prediction that $\bar{Y}$ may either increase or decrease with amplitude depending on the incidence angle. They also confirm the theory's prediction that redeposition scales with the square of the amplitude over the wavelength, and are generally in excellent quantitative agreement with theory.

[1] R.M. Bradley, G. Hobler, submitted for publication.
[2] G. Hobler, Nucl. Instrum. Meth. B 96 (1995) 155.

O 13.4 Mon 16:00 GER 38

MeV-SIMS: mass spectrometry with ultra-fast projectiles — •Lars Breuer[1], Tobias Heckhoff[1], David Theuner[1], Frieder Koch[2], and Andreas Wucher[1] — [1]Universität Duisburg-Essen — [2]GSI Helmholtzzentrum für Schwerionenforschung

While secondary ion mass spectrometry has become a standard tool in surface analysis, it still offers multiple challenges. While ionization probabilities are usually fairly low and may be altered by the chemical environment of the target surface, fragmentation of molecules introduces even more experimental challenges. Therefore, better understanding of the underlying processes and methodology improvement is an ongoing topic of research. Here, we present strategies developed to shed light on the fundamental processes in sputtering of different materials from metals and insulators to organic samples by tuning the contribution of nuclear and electronic sputtering. For that purpose, a time-of-flight spectrometer has been coupled to the M-Branch of the UNILAC at GSI in Darmstadt, using swift heavy ions as projectiles.

By laser post-ionization not only secondary ions are accessible but their neutral counterparts as well to enable us to gain insight into sputtering and ionization under extreme conditions.

O 13.5 Mon 16:15 GER 38

A new material science target station for swift and highly charged ions at CRYRING@ESR — •Kevin Vomschee[1], Michael Wagner[2], Nils Ulrich[2,3], Frieder Koch[2], Sadra Kour[1], André Maas[1], Christina Trautmann[2,3], Marika Schleberger[1], and Lars Breuer[1] — [1]Univ. Duisburg-Essen — [2]GSI Helmholtzzentrum für Schwerionenforschung — [3]Technische Univ. Darmstadt

This contribution describes the new target station MSS@CRYRING ("Material Science Station at CRYRING") operated at GSI. The new setup at the storage ring CRYRING allows the irradiation of samples with highly charged ions up to completely stripped uranium (U^{92+}) with full control over the kinetic energy of the projectile between keV and GeV. This allows the investigation of the specific effect of the kinetic and potential energy. The latter is dissipated in a very shallow volume upon impact while at high kinetic energies the entire bulk material is irradiated.
We report on results from the first beam times using the extracted beam at the new target station. For testing the setup, polymer films were irradiated with $^{107}Ag^{47+}$ at a kinetic energy of 5.9 MeV/u. Applying track etching techniques the number of ions per cm^2 was analyzed using scanning electron microscopy. Comparing these results with the number of ions extracted from the storage ring as deduced from a DC-transformer and a Schottky detector gives an ion transmission of 53.7 % and a maximum flux of $3 \cdot 10^7$ cm^{-2} per pulse.

O 13.6 Mon 16:30 GER 38

Compact Electron Beam Ion Source — •Daniel Thima[1], Matthias Werl[1], Gabriel Lukas Szabo[1], Paul-Friedmar Laux[2], Mike Schmidt[2], Günter Zschornack[2], and Richard Arthur Wilhelm[1] — [1]TU Wien, Institute of Applied Physics, Vienna, Austria — [2]D.I.S Germany GmbH, Dresden, Germany

In many modern fields of research, such as plasma and atomic physics, material science or astrophysics, highly charged ions play an important role. Research with highly charged ions relies strongly on stable ion sources, providing long-term operation with the low output currents in standard devices. Typically, these devices are heavy, stationary machines such as electron cyclotron resonance ion sources or electron beam ion sources (EBIS), sometimes even relying on cryogenic magnetic systems.

Gaining portability by downsizing an EBIS has been pursued recently by a commercial supplier. With only 30 cm in length and using in-vacuum mounted magnets, the resulting prototype EBIS fits onto almost any ultra high vacuum chamber, needing only a single CF40 port. An included Wien filter allows separation of produced ions based on their charge state and mass.

We are currently characterising this compact EBIS in our laboratory, focusing on ion output current. Here, we present our setup and the results of first measurements.

O 13.7 Mon 16:45 GER 38

On the path to ion based pump-probe experiment: generating picosecond keV Ne^+ ion pulses from a cooled supersonic gas beam — •Lukas Kalkhoff, Marika Schleberger, Klaus Sokolowski-Tinten, Andreas Wucher, Alexander Golombek, and Lars Breuer — University Duisburg-Essen, Duisburg, Germany

The dynamics triggered by the impact of an ion onto a solid surface has been explored mainly by theoretical modeling or computer simulation to date. Results indicate that the microscopic non-equilibrium relaxation processes triggered by the interaction of the ion with the solid occur on a (sub-)picosecond time scale. A suitable experimental approach to these dynamics therefore requires a pump-probe method with an appropriate time resolution. Our experiments have successfully used laser photoionization of a supersonic beam of cooled noble gas atoms at $T_{atoms} \simeq 4$ K in combination with a Wiley-MacLaren ion buncher. The measured distribution of the arrival time of individual Ne^+ ions impinging on the surface of a fast microchannel plate with a kinetic energy of 4 keV gives a full width at half maximum of the ion pulse of $t_{ion} = 130$ ps. A more detailed analysis shows that this pulse width is only an upper limit related to the detection limit of the electronics. The true pulse width results from extrapolation of our data and is $t_{ion} = 18 \pm 4$ ps. This opens the door to pump-probe experiments with keV ions with a time-resolution in the picosecond range.

O 13.8 Mon 17:00 GER 38

Generation of pulsed ions using ultrafast electrons — Marius Constantin Chirita Mihaila, Gabriel Lukas Szabo, Alexander Sagar Grossek, and •Richard Arthur Wilhelm — TU Wien, Institute of Applied Physics, 1040 Vienna, Austria

Ultrafast physics is a very active research field where high temporal and spatial resolution provides unprecedented structural information in material science.

Here, we describe the development of a new technique that allows the creation of pulsed ions using ultrafast electrons. The general technique of using picosecond ion pulses to study novel time-resolved processes in materials will be hugely impactful and aims at investigating ultrafast phenomena that are intractable with pump-probe measurements using pulsed electrons and lasers. However, the use of pulsed ions has been limited by the complexity of achieving short pulse lengths at the sample plane.

The experimental setup features a Ti: Sapphire laser that triggers femtosecond electron pulses from a low-workfunction cathode. The pulsed electrons then propagate through a miniaturized ion source and generate pulsed ions. Current challenges of preserving a short ion pulse length upon transport to the sample plane and prospects of pump-probe measurements with ultrafast ions are discussed.

O 14: Nanostructures at Surfaces (joint session O/CPP)

Time: Monday 15:00–17:45 Location: GER 39

O 14.1 Mon 15:00 GER 39

Tailoring Stone-Wales transitions in Ti_2O_3 honeycombs with alkaline earth metals — •Martin Haller, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, Von-Danckelmann-Platz 3, 06120 Halle, Germany

In 2013 the first 2D oxide quasicrystal (OQC) has been discovered in thin Ba-Ti-O films [1]. It shows a twelvefold diffraction pattern that is incompatible with lattice periodicity. In real space it can be described by squares, triangles and rhombus tiles. Just recently, the atomic structure has been solved [2,3]. The essence are Ti_nO_n ring structures with n = 4, 7 and 10. These evolve by Stone-Wales transitions from a pure honeycomb network [4]. The transformations are stabilized by alkaline earth metal ions and their associated dipole and can be controlled by the alkaline earth metal coverage. Here we investigate the basic steps of individual Stone-Wales transformations with LEED and STM for ultra-low coverages deposited onto a Ti_2O_3 honeycomb on a close-packed metal surface. The transformations to ring structures with n = 4, 5 and 7 are monitored and related to the formation of square and triangle tilings.

[1] S. Förster et al., Nature 502, 215 (2013)
[2] S. Schenk et al., Nat. Comm., accepted, (2022)
[3] E. Cockayne et al., Phys. Rev. B 93, 020101 (2016)
[4] S. Wang et al., Nanoscale 11, 2412 (2019)

O 14.2 Mon 15:15 GER 39

Formation of an extended quantum dot array driven and auto protected by an atom thick h-BN layer — •Joel Deyerling[1], Ignacio Piquero-Zulaica[1], Mustafa A. Ashoush[2], Knud Seufert[1], Mohammad A. Kher-Elden[2], Zakaria M. Abd El-Fattah[2], and Willi Auwärter[1] — [1]Physics Department E20, Technical University of Munich, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Physics Department, Faculty of Science, Al-Azhar University, Nasr City, Cairo E-11884, Egypt

Fabricating nanoarchitectures to confine two dimensional nearly free electrons on crystalline surfaces by tip manipulation with a scanning tunneling microscope (STM) or by applying supramolecular chemistry principles yields diverse artificial electronic structures. These electronic states are prone to scattering by adsorbates making them extremely susceptible to the environment. Nonetheless, little attention has been given to their protection, e.g., by an inert overlayer.

Here, we show that a quasi-hexagonal CuS nanoporous network can be formed at the h-BN/Cu(111) interface by thermally-induced sulfur segregation from the Cu(111) bulk. The growth and structure is characterized by STM and X-ray photoemission spectroscopy. We demonstrate by employing STM and scanning tunneling spectroscopy that within the pores of the network the surface state of Cu(111) as well as the image potential states of h-BN/Cu(111) are confined, effectively creating arrays of quantum dots with well-defined sizes that are covered by an inert h-BN overlayer.

O 14.3 Mon 15:30 GER 39

First-principles investigation of doped borophene quantum dots as donor materials for solar cell applications — •Rachana Yogi, Vaishali Roondhe, and Alok Shukla — Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

Because of fast-depleting fossil fuel reserves, there is an urgent need for harvesting alternative sources of energy. We present a first-principles atomistic study of borophene quantum dots (BQDs) B35 and B36 for their possible utilization in solar-cells. The pristine-BQDs are doped by C, N, and O atoms, and find that they have bowl-like structures in the ground state. The electronic and optical properties of pristine-BQDs, and doped-BQDs are investigated. The chemical potentials of several of these BQDs are slightly higher than that of popular solar-cell acceptor system PC71BM, they will act as electron donors in a PC71BM-based solar-cell. The calculated values of the open-circuit voltage corresponding to PC71BM and BQD-based device indicate efficient electron injection from the BQDs to PC71BM. O-doped B36-QD and B35-QD have the highest value of short-circuit current density attributed to their reduced HOMO-LUMO gap and high HOMO energy levels as compared to all other considered doped systems further enhancing the photoelectric properties. The power conversion efficiency of doped-BQDs exhibits significant improvement. The efficiency of O-doped B36-QD is maximum due to its high electron injection rate in PC71BM. Present calculations show that adding a foreign atom in BQD makes it a suitable candidate for high-performance solar-cells.

O 14.4 Mon 15:45 GER 39

Electrospray Depositions of a Spin-Crossover Active Iron(II) [2×2] Grid Complex on Ag(111) with Different Landing Energies — •Dennis Meier[1], Benedikt Schoof[1], Joachim Reichert[1], Nithin Surayadevara[2], Andreas Walz[1], Annette Huettig[1], Hartmut Schlichting[1], Mario Ruben[2], Anthoula C. Papageorgiou[1,3], and Johannes V. Barth[1] — [1]Technical University of Munich, Germany — [2]Karlsruhe Institute of Technology, Germany — [3]National and Kapodistrian University of Athens, Greece

Chiral spin-crossover (SCO) complexes are intriguing building blocks for innovative magneto-optical nanoarchitectures.[1] Such an Fe(II) [2×2] grid complex was deposited in ultra-high vacuum with electrospray controlled ion beam deposition (ES-CIBD)[2] on Ag(111) and investigated by scanning tunnelling microscopy. Low landing energy ($<$ 3 eV/z) resulted in clusters and single molecules. Higher landing energies ($>$ 3 eV/z) led to coordination bond cleavage and a rich variety of self-assembled surface networks forming from the grid fragments. Applying established on-surface synthesis methodology employing the possible constituents of these networks (ligands and Fe atoms) reproduced only a part of them. It is thus proposed that ES-CIBD provides an unexpected route to novel on-surface coordination network synthesis.

[1] N. Suryadevara et al. *Chem. Eur. J.* 2021, **27**, 15172.
[2] A. Walz, K. Stoiber, A. Huettig, H. Schlichting, J. V. Barth, *Anal. Chem.* 2022, **94**, 7767.

O 14.5 Mon 16:00 GER 39

Giant confinement of surface electrons in a two-dimensional metal-organic porous network — •Lu Lyu[1], Tobias Eul[1], Wei Yao[1], Zakaria M. Abd El-Fattah[2], Mostafa Ashoush[2], Ignacio Piquero-Zulaica[3], Johannes V. Barth[3], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,4] — [1]Department of Physics, University of Kaiserslautern, Germany. — [2]Physics Department, Faculty of Science, Al-Azhar University, Egypt. — [3]Physics Department E20, Technical University of Munich, Germany — [4]Institute of Physics, Johannes Gutenberg University Mainz, Germany.

Two-dimensional metal-organic porous networks (2D-MOPNs) are highly flexible nano-architectures for exploring the quantum confinement of surface electrons on noble metals. So far, 2D-MOPNs have been predominantly studied for the confinement of occupied Shockley-type surface states (SS). In contrast, the confinement of excited surface states, such as image potential states (IPSs), remains elusive. In this work, we apply two-photon photoemission to investigate the band dispersion of the first image-potential state (n = 1 IPS) in a Cu-T4PT nanoporous network on Cu(111). We find the formation of a Bloch-like band structure with a substantially increased effective band mass of the IPS ($>$ 150 %). In contrast, the effective band mass of the SS remains almost unchanged ($<$ 3%). This band renormalization of the IPS can be attributed to the spatial distribution of its charge density perpendicular to the surface, which reveals the highest density at the vertical adsorption position of the T4PT backbone. This coincidence is responsible for the giant confinement.

O 14.6 Mon 16:15 GER 39

Modification of Single-Layer Organometallic Networks: from Ag-Bridged to Cu-Bridged Alkynyl Metal-Alkynyl Linkages on Ag(111) Surfaces — •Wenchao Zhao, Felix Haag, Ignacio Piquero-Zulaica, Yi-Qi Zhang, Francesco Allegretti, Biao Yang, and Johannes V Barth — Physics Department E20, Technical University of Munich, 85748 Garching, Germany

The metal-exchange reaction, is of importance for the advanced preparation of functional metal-organic frameworks for various applications[1]. Notably, building two-dimensional organometallic networks (OMNs), can provide versatile nanoarchitectures for potential application in nanodevice[2,3]. Although various OMNs have been constructed with molecular building blocks by abstracting surface metal atoms, the degree of success is often individual and substrate-dependent. Thus metal-exchange reactions hold promise for multiple production by modification and functionalization of OMN templates. Here, we demonstrate the modification of a single-layer OMN by metal-exchange reaction. By introducing external Cu atoms into the alkynyl-Ag OMN[3], we successfully synthesized in situ a highly ordered alkynyl-Cu OMN on a Ag(111) surface. While maintaining a similar lattice periodicity and pore morphology, it possesses higher thermal stability, guaranteeing higher robustness for possible applications. Reference. 1. M.-M. Xu et al., Coord. Chem. Rev. 2020, 421, 213421. 2. D. Ecija et al., Acc. Chem. Res. 2018, 51, 365-375. 3. Y.-Q. Zhang et al., J. Am. Chem. Soc. 2019, 141, 5087-5091

O 14.7 Mon 16:30 GER 39

Structure Formation in Ceramic Thin Films with Hybrid Molecular Dynamics — •Nydia Roxana Varela Rosales and Michael Engel — Institute for Multiscale Simulation, University of Erlangen-Nürnberg, Cauerstraße 3, 91058 Erlangen, Germany

How can we model and predict ceramic thin films? Highest accuracy is achieved with ab-initio quantum mechanical methods. But these methods are not suitable for large systems including their phase transformations. Atomistic modeling with molecular dynamics and Monte Carlo simulations reaches large system sizes but require sophisticated tailored interaction potentials. Here, we develop and apply a coarse-grained simulation method for structure formation in thin films. Our method considers the chemical bond network of the ceramics explicitly to simplify the complexity of the simulation and to reach high simulation speeds and large system sizes. Of particular interest are (quasi-)crystalline ceramic thin films recently discovered in experiments of (Ba/Sr)-Ti-O perovskites. Solely by considering the extrinsic topology of the tiles and utilizing a harmonic interaction potential, we reproduce the appearance of approximants of the dodecagonal quasicrystals, which was also predicted by ab-initio simulations. Our work highlights the role of bond network topology in understanding complex thin film structures without a need for reliance on quantum simulation methods.

O 14.8 Mon 16:45 GER 39

A Holistic Characterisation of Bi Thin Films on Au(111) — •Pablo Vezzoni Vicente[1], Tobias Weiss[1], Marc Gonzalez-Cuixart[4], Dennis Meier[1], Benedikt Klein[2], David Duncan[2], Ezequiel Tosi[3], Paolo Lacovig[3], Silvano Lizzit[3], Johannes Barth[1], Peter Feulner[1], and Francesco Allegretti[1] — [1]Physics Department E20, Technische Universität München, Germany — [2]2I09 beamline, Diamond Light Source, United Kingdom — [3]3SuperESCA beamline, Elettra Synchrotron, Italy — [4]4IMDEA Nanociencia, Spain

We present a comprehensive analysis of the long-range ordered, coverage-dependent phases of Bi epitaxially grown on a Au(111) surface in UHV, from the sub-monolayer $(\sqrt{37} \times \sqrt{37})R25.3^\circ$ Kagome lattice up to few-layer Bi(110) thin films. Particular focus is devoted to the sub-monolayer, high-coverage $(p \times \sqrt{3})$ phase, paving the way to its use as a buffer layer for epitaxial growth with tunable geometry and low electronic interaction.

Our work clarifies and expands the current literature reports, specifically on the complex $(p \times \sqrt{3})$ phase. The wide range of analysis techniques used, including Low-Energy Electron Diffraction (LEED), Photo-Electron Spectroscopy (XPS, UPS), Temperature Programmed Desorption (TPD), Scanning Tunneling Microscopy and Spectroscopy (STM, STS), and X-ray Standing Waves (XSW), yields an unprecedented understanding of the system's structural and electronic properties.

O 14.9 Mon 17:00 GER 39

Analytical electron microscopy of nanostructured vanadium dioxide — •Vlastimil Křápek[1], Jan Krpenský[1,2], Michal Horák[1], Katarína Rovenská[1], Peter Kepič[1], Tomáš Šikola[1], Filip Ligmajer[1], and Andrea Konečná[1] — [1]Brno University of Technology, Czechia — [2]CIC nanoGUNE, San Sebastián, Spain

Vanadium dioxide (VO_2) is a phase-changing material exhibiting temperature-induced metal-insulator transition (MIT) around 340 K. A rather low transition temperature makes VO_2 a suitable material for active nanophotonics, e.g., switchable optical metasurfaces. Such applications require nanostructuring of VO_2 thin films. Here we study the possibility to employ focused ion beam (FIB) milling for the nanofabrication and its impact on the properties of resulting nanostructures.

Taking the VO_2 thin film with experimentally verified MIT, we utilized FIB milling with Ga ions to fabricate V-shaped lamella of the thickness between 0 and 250 nm, which was subsequently transferred onto a heating chip for transmission electron microscopy and analyzed with analytical electron microscopy: high-resolution imaging, energy-dispersive X-ray spectroscopy, and temperature-dependent electron energy loss spectroscopy. We observed a porous character of the pristine material, a coexistence of several crystal structures, negligible contamination with Ga ions, and a variation of stoichiometry with the thickness of the lamella, with the thinnest parts composed of VO and V_2O_3.

O 14.10 Mon 17:15 GER 39

Tuning Nanoporous Au Film Formation via High Voltage Electrolysis — •Evelyn Artmann[1], Lukas Forschner[1], Konstantin M. Schüttler[2], Mohammad Al-Shakran[1], Timo Jacob[1], and Albert K. Engstfeld[1] — [1]Institute of Electrochemistry, University of Ulm, Germany — [2]Institute of Surface Chemistry and Catalysis, University of Ulm, Germany

Nanoporous Au (NPG) films have different properties compared to the bulk material, which opens up new areas of application, such as (electro)catalysis. Usually, NPG films are prepared by dealloying. One disadvantage of this method is that residues of the precursor alloy guest metal can remain in the resulting NPG film, which can have a decisive influence on the electrocatalytic activity of the NPG film.

In this work we report on the preparation of NPG films by high voltage electrolysis (Chem. Phys. Chem., 22 (2021) 2429). In this process, a Au oxide film is first formed on the Au substrate by applying a high positive voltage (between 100 and 540 V), which can subsequently be reduced to NPG. The Au oxide as well as NPG films were characterized by electrochemical methods, as well as (cross-section) SEM and XPS measurements.

Possibilities to selectively modify the resulting NPG films by tuning experimental parameters such as the applied voltage, and electrolyte temperature during HV electrolysis, or the electrolysis time, were systematically investigated. The influence of the reduction method (electrochemical or by H2O2) on the final film structure is discussed.

O 14.11 Mon 17:30 GER 39

Evolution of the Si-Au alloy: from the gold (110) substrate to silicon nanoribbons — •Ekaterina Tikhodeeva[1], María E Dávila[2], Paola De Padova[3], Gay Le Lay[4], Marina Baidakova[5], Evgeniya Lobanova[5], Jaime Sanchez-Barriga[6], Dmitrii Smirnov[6], and Manuel Izquierdo[1] — [1]European XFEL, Schenefeld, Germany — [2]CSIC, Madrid, Spain — [3]Consiglio Nazionale delle Ricerche, Rome, Italy — [4]Aix-Marseille Université, Marseille, France — [5]Saint Petersburg, Russia — [6]Helmholtz-Zentrum Berlin, Berlin, Germany

The development of the Si-Au alloy was investigated on the path from the gold single crystal surface to silicon nanoribbons (SiNR). Si sub-monolayers were deposited on the missing row reconstructed Au(110) substrate. At various stages of evaporation, low-energy electron diffraction (LEED) patterns were recorded to refine the surface geometry. The arrangement of the Si atoms has been correlated with the missing row orientation. The recovery of the Au(1x1) reconstruction, as well as the gradual transition from surface alloy to SiNRs were explored. In parallel with LEED, photoelectron spectroscopy was used to clarify the atom distribution. The profiles of the Au 4f and Si 2p core levels were deconvoluted and analyzed at all stages of Si deposition. The appearance of a new low kinetic energy component was noticed in the Au 4f spectra. It is related to the Si-Au bond and indicates a strong interaction between them. The Si core levels exhibit up to three components corresponding to the different chemical environments.

O 15: Spins on Surfaces at the Atomic Scale II

Time: Monday 15:00–18:00 Location: REC C 213

O 15.1 Mon 15:00 REC C 213

Electron-spin resonance atomic force microscopy — •Lisanne Sellies, Raffael Spachtholz, Philipp Scheuerer, and Jascha Repp — University of Regensburg, Regensburg, Germany

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

ESR-AFM allows to measure ESR signals with a sub-nanoelectronvolt energy resolution, as we demonstrated for pentacene on thick NaCl films. Thereby, molecules only differing in their isotopic configuration can be distinguished. Moreover, due to the minimally invasive nature of the ESR-AFM technique, the electron spins of pentacene can be coherently manipulated over tens of microseconds. After introducing ESR-AFM, recent results obtained by this technique will be presented.

References: [1] Köhler et al. (1993). Nature, 363(6426), 242-244. [2] Wrachtrup et al. (1993). Nature, 363(6426), 244-245. [3] Peng et al. (2021). Science, 373(6553), 452-456.

O 15.2 Mon 15:15 REC C 213

Coherent spin dynamics in a single atom hyperfine system — •Lukas Veldman, Laëtitia Farinacci, Evert Stolte, Mark Canavan, and Sander Otte — TU Delft, Delft, The Netherlands

The combination of electron spin resonance (ESR) with scanning tunneling microscopy (STM) has opened up the possibility to investigate the interaction between electrons and nuclei in individual atoms on a surface [1]. Recently, we showed that for TiH atoms on MgO the hyperfine interaction is highly anisotropic and contains information on the groundstate orbital of the atom [2]. In this work, we go to the low field regime where electron and nuclear states hybridize. We use DC voltage pulses [3] to spin pump both the electron and the nuclear spin [4]. We measure the coherent oscillations of the electron spin driven by the hyperfine interaction. These measurements open the door to controlled spin manipulation of nuclear spins in single atoms.

[1] Willke et al. Science 362 (2018)
[2] Farinacci et al. Nano Letters (2022)
[3] Veldman et al. Science 372 (2021)
[4] Yang et al. Nature Nanotechnology 13 (2018)

O 15.3 Mon 15:30 REC C 213

Quantum coherence of single atomic S = 1/2 spins on ultra-thin insulating layers — Hong Bui[1,2], We-Hyo Seo[1,2], Yu Wang[1,2], Andreas Heinrich[1,2], and •Soo-Hyon Phark[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul

03760, Korea — [2]Department of Physics, Ewha Womans Universtiy, Seoul 03760, Korea

A scanning tunneling microscope (STM), when combined with electron spin resonance (ESR), provides a solid-state platform of atomic scale spin qubit. However, its quantum coherence is considerably limited by couplings with metallic substrate and tunneling electrons. Here we report a study on the quantum coherence of single Ti atomic spins ($S = 1/2$) on two- (2ML) and three- (3ML) monolayer-thick MgO on Ag(100) using pulsed-ESR equipped in a STM at 0.4 K. We were able to drive the coherent rotations of the spin on the 3ML-MgO with a Rabi rate (Ω) up to 100 MHz, which is an order faster than that on the 2ML-MgO. Coherence time (T2) from Hahn-echo measurement revealed the role of the tunneling electrons, resetting the state of a Ti spin with a probability of 0.15/electron, which is the same for Ti spins on both 2ML- and 3ML-MgO. Of more interesting is the zero current T2 of 2 microsec on 3ML-MgO, about 5 times longer than that on 2ML-MgO, emphasizing the importance of decoupling the spin from the metallic substrate as well as tunneling electrons. Such considerable improvements in Ω and T2 are promising for high fidelity quantum gate operations to a Ti spin qubit, further brightening a way to raise the on-surface spin qubits on a stage of the quantum-coherent applications.

O 15.4 Mon 15:45 REC C 213

Certifying entanglement of spins on surfaces using ESR-STM — •Yelko del Castillo[1,2] and Joaquín Fernández-Rossier[1] — [1]International Iberian Nanotechnology Laboratory (INL), Av. Mestre José Veiga, 4715-330 Braga, Portugal — [2]Centro de Física das Universidades do Minho e do Porto, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal

We propose a protocol to certify the presence of entanglement in artificial on-surface atomic and molecular spin arrays using electron spin resonance carried by scanning tunnel microscopes (ESR-STM). We first generalize the theorem that relates global spin susceptibility as an entanglement witness to the case of anisotropic Zeeman interactions, relevant for surfaces. We then propose a method to measure the spin susceptibilities of surface-spin arrays combining ESR-STM with atomic manipulation. Our calculations show that entanglement can be certified in antiferromagnetically coupled spin chains using state of the art spectral resolution of ESR-STM magnetometry.

O 15.5 Mon 16:00 REC C 213

Ultrafast dynamics of magnetic adatoms on MgO — •Lukas Arnhold[1], Daria Sostina[2], Nicolaj Betz[1], Susanne Baumann[1], Philip Willke[2], and Sebastian Loth[1] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Karlsruhe Institute of Technologies, Physikalisches Institut, Karlsruhe, Germany

The utilization of single magnetic atoms as qubits requires detailed understanding of their energy levels and the associated time-scales, ideally also those of excited states. Ever since coherent driving of a single spin in the junction of a scanning tunneling microscope has been shown [1], the technique of ESR-STM has been established and used for example to perform qubit operations, as well as, to address multiple qubits [2]. Besides the technique of electron spin resonance, quantum stochastic resonance measurements offer new insights into a system's energy transition cycles, or in other words, it's associated time-scales [3]. Applying this measurement scheme onto ESR active adatoms on a MgO substrate, gives access to additional manipulation pathways and allows for further understanding and mastery of coherent spin manipulation.

[1] Baumann, Susanne et al. 'Electron paramagnetic resonance of individual atoms on a surface.' Science 350 (2015): 417 - 420.

[2] Phark, Soo-Hyon et al. 'Double Electron Spin Resonance of Engineered Atomic Structures on a Surface.' arXiv:2108.09880, 2021.

[3] Haenze, Max et al. 'Quantum Stochastic Resonance of individual Fe atoms.' Sci. Adv. Vol 7, Issue 33 (2021).

O 15.6 Mon 16:15 REC C 213

All-electrical driving and probing dressed states of a single spin on surface — •Hong Bui Thi[1,2], Christoph Wolf[1,3], Yu Wang[1,3], Masahiro Haze[1,4], Yi Chen[1,3], Yujeong Bae[1,2], Andreas Heinrich[1,2], and Soo-Hyon Phark[1,3] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Korea — [2]Department of Physics, Ewha Womans University, Seoul 03760, Korea — [3]Ewha Womans University, Seoul 03760, Korea — [4]The Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan

We demonstrate the creation of dressed states of a single electron spin localized on a surface by using a resonant radio-frequency field in a scanning tunneling microscope. Owing to the unique sub-nm probe-sample geometry field strengths as high as 1 GV/m can be achieved at a bias of the radio-frequency field below 100 mV. Magnetic resonance of a single spin in such a cavity is a direct consequence of coupling between the atomic dipole moment and driving electric field, resulting in the dressing of the atomic states. The read-out of these dressed states is facilitated in an all-electrical fashion by a weakly coupled probe spin. Our work highlights the strength of the atomic-scale geometry inherent to the scanning tunneling microscope in terms of the creation and control of dressed states, which are known to provide decoherence-free subspaces critical to the creation of long-lived quantum states.

O 15.7 Mon 16:30 REC C 213

Surface spins as quantum bits - a simulation perspective — Jose Reina Gálvez[1], Nicolas Lorente[2], and •Christoph Wolf[1] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, South Korea — [2]Materials Physics Center, San Sebastian, Spain

Spins localized at or close to a clean surface have emerged as systems of interest in quantum nanoscience. They can be tailored to a desired spin state, manipulated to form structures with designed interactions and as of recent have been used to implement basic quantum logic operations - a control-NOT gate - in a scanning tunneling microscope (STM). In this work we want to explore quantum coherent phenomena of surface spins from a computational perspective. Since surface spins interact rather strongly with the environment, we performed open quantum systems calculations. First, we will show how electron-electron double resonance can be understood by solving the time-dependent Schrodinger equation under continuous and pulsed radio-frequency driving. Using the same prototypical system of two coupled electron spins we also show how the AC Stark effect manifests itself as Autler-Townes doublets and Mollow triplets. To go one step further, we use our recently developed approach to explicitly calculate the current present in the STM experiment using the non-equilibrium Green's functions formalism. These simulations show how the current plays a dual role in these systems by driving quantum transitions but also limiting quantum coherence. Our simulations outline realistic expectations for quantum coherent surface spin systems and their prospective applications.

O 15.8 Mon 16:45 REC C 213

A non equilibrium Green's Function formalism applied to STM/ESR experiments — •Jose Reina-Galvez[1], Nicolas Lorente[2], and Christoph Wolf[1] — [1]Center for Quantum nanoscience, Seoul, South Korea — [2]Centro de Fisica de Materiales, San Sebastian, Spain

The demonstration of reproducible single-atom and single-molecule electron spin resonance (ESR) in a STM junction opened new possibilities in the analysis of surface science at the atomic scale. Recent experiments have demonstrated quantum-coherent Rabi oscillations and even the implementation of a quantum logic operation: a CNOT gate.

Here, we want to focus on the theory we developed to reproduce some relevant results in the field. Our theoretical framework uses open quantum systems formalism in combination with non equilibrium Green's Function technique. It consists of a quantum impurity connected to a polarized STM tip and an isolated surface, both considered as fermionic baths. The time dependent bias voltage used in the experiments is introduced in the hopping terms. These hoppings are driving the electron transitions from the baths to the quantum impurity which uses a modified Anderson impurity model with localized electronic states, a Coulomb repulsion term and a Zeeman term.

Our model is general, allowing to connect an arbitrary number of localized spins with the transport spin. We will demonstrate how driving the system on resonance modifies the population and the calculated true current through the many-body impurity which can be directly compared to the experiment.

O 15.9 Mon 17:00 REC C 213

Microscopic theory of spin-relaxation of a single Fe adatom coupled to substrate vibrations — •Haritz Garai-Marin[1,2], Manuel dos Santos Dias[3,4,5], Samir Lounis[3,4], Julen Ibañez-Azpiroz[6,7], and Asier Eiguren[1,2,8] — [1]Physics Department, University of the Basque Country UPV/EHU, Bilbao, Spain — [2]Donostia International Physics Center, Donostia, Spain — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Jülich, Germany — [4]Faculty of Physics, University of Duisburg-Essen & CENIDE, Duisburg, Germany — [5]Scientific Com-

puting Department, STFC Daresbury Laboratory, Warrington, United Kingdom — [6]Centro de Física de Materiales CSIC-UPV/EHU, Donostia, Spain — [7]IKERBASQUE Basque Foundation for Science, Bilbao, Spain — [8]EHU Quantum Center, University of the Basque Country UPV/EHU

Understanding the spin-relaxation mechanism of single adatoms is an essential step towards creating atomic magnetic memory bits or quantum bits. Here we present a theory to study the role of electron-phonon coupling by combining *ab-initio* electronic and vibrational properties with the multiplet many-body nature of atomic states. Our calculations reproduce the millisecond spin lifetime measured on Fe adatoms on MgO/Ag(100), which demonstrates that the essential features of the spin-phonon coupling are successfully captured. We show a clear fingerprint for experimentally detecting a localized spin-phonon excitation and we show how the atomic interaction with the environment should be tuned in order to enhance the magnetic stability.

O 15.10 Mon 17:15 REC C 213

Electron spin resonance of individual magnetic molecules on surfaces — •Wantong Huang[1], Máté Stark[1], Paul Greule[1], Daria Sostina[2], David Collomb[1], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], and Philip Willke[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology, Karlsruhe, Germany

Single molecular magnets which consist of one central metal ion surrounded by ligands are promising building blocks for nanoscale spintronics and future quantum devices. The recent development of scanning tunnelling microscopy (STM) combined with electron spin resonance (ESR) constitutes here a powerful technique to image and coherently control individual molecular spins on surfaces [Zhang et. al, Nat. Chem. 14, 59 (2022); Willke, ACS Nano, 15, 11, 17959 (2021)]. Here, we explore the magnetic properties and spin dynamics of iron phthalocyanine (FePc) molecules adsorbed on magnesium oxide (MgO) grown on Ag(100). We investigate the magnetic properties of different FePc by scanning tunneling spectroscopy and ESR-STM. Such molecular magnetic structures provide a versatile platform to study complex magnetic interactions and atomic-scale spin dynamics.

O 15.11 Mon 17:30 REC C 213

Orbital and spin excitations of hydrogenated titanium modulated by electric field — •Daria Sostina[1], Lukas Arnhold[2], Nicolaj Betz[2], Susanne Baumann[2], Philip Willke[3], Wolfgang Wernsdorfer[3], and Sebastian Loth[2] — [1]Institute of Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [3]Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

The goal for coherent control of individual spins on surfaces has prompted the development of new local probe techniques such as a combination of electron spin resonance (ESR) with scanning tunneling spectroscopy (STM). Yet, the excitation mechanism of ESR in STM is not conclusively determined. [Baumann et.al, Science 350, 6259, 2015, Ferron et. al, Phys. Rev. Research 1, 033185 (2019)]. Here we study a higher order orbital excitation of hydrogenated titanium complexes positioned on the oxygen site of the MgO surface. We observe a strong dependence of its excitation energy on the electric field generated by the STM tip. At the same time an ESR transition on that TiH exhibits a shift with the DC bias voltage applied to the junction which was attributed to a change in g-factor of the complex [Kot et. al, arXiv 2209.10969, 2022]. The ability to tune orbital and spin excitations by means of electric fields gives further insight on new pathways for electrical control of single spins centers on surfaces.

O 15.12 Mon 17:45 REC C 213

Lanthanide atoms on MgO(100)/Ag(100) as Candidate for Single-Atom-Qubits — Stefano Reale[1,2,3], Aparajita Singha[1,2,4], Safa L. Ahmed[1,2], Denis Krylov[1,2], Luciano Colazzo[1,2], Christoph Wolf[1,2], Carlo S. Casari[3], Alessandro Barla[5], Edgar Fernandez[6], Francois Patthery[6], Marina Pivetta[6], Stefano Rusponi[6], Harald Brune[6], and •Fabio Donati[1,2] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Republic of Korea — [2]Department of Physics, Ewha Womans University, Republic of Korea — [3]Department of Energy, Politecnico di Milano, Italy — [4]Max Planck Institute for Solid State Research, Germany — [5]Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR), Italy — [6]Institute of Physics, Ecole Polytechnique Federale de Lausanne, Switzerland

Lanthanide atoms on surfaces are an exceptional platform for atomic-scale magnetic information storage [Science 352, 318 (2016)]. However, their potential as qubits is yet unexplored. Here we combine x-ray absorption spectroscopy and scanning tunneling microscopy (STM) with density functional theory and multiplet calculations to estimate the performance of Er and Tm on MgO(100)/Ag(100) as spin qubit candidates. For both atoms, we infer a magnetic ground state that is suitable for quantum coherent operations. By adapting the piezoelectric model of electron spin resonance (ESR)-STM [Science Advances 6, eabc5511 (2020)] to the case of lanthanide atoms, we predict a detectable signal and a higher Rabi rate compared to the systems studied up to date [S. Reale et al., accepted in Phys. Rev. B].

O 16: Ultrafast Electron Dynamics at Surface and Interfaces II

Time: Monday 15:00–17:30 Location: TRE Phy

O 16.1 Mon 15:00 TRE Phy

Time Resolved Photoemission Study of the Charge Transfer Dynamics in Rutile $TiO_2(110)$ for CO Photooxidation to CO_2 — •Helena Gleissner[1,2,3], Michael Wagstaffe[2], Lukas Wenthaus[4], Simon Chung[2], Steffen Palutke[4], Siarhei Dziarzhytski[4], Dmytro Kutnyakhov[4], Michael Heber[4], Günter Brenner[4], Harald Redlin[4], Heshmat Noei[1,2], and Andreas Stierle[1,2,3] — [1]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [2]Center for X-ray and Nano Science (CXNS), Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [3]Fachbereich Physik Universität Hamburg, Hamburg, Germany — [4]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany

In a pump-probe experiment at the free electron laser in Hamburg (FLASH) we gained insight into the ultrafast charge transfer on rutile $TiO_2(110)$ during CO oxidation to CO_2. Pumped with a 770 nm optical laser and probed with 643 eV FEL soft x-rays we monitored the changes in the O 1s and Ti 2p core levels on a picosecond timescale using time-resolved photoemission spectroscopy.

We find that oxygen gets activated and reacts with CO to CO_2 in 0.2 ps up to 1 ps after the laser excitation. A complementary study found that the CO oxidation on anatase $TiO_2(101)$ takes place between 1.2 and 2.8 ps after irradiation with an ultrashort laser pulse.[1]

[1] Wagstaffe, M. et al. ACS Catal. 10, 13650-13658 (2020).

O 16.2 Mon 15:15 TRE Phy

Transient Absorption Spectroscopy of NiO — •Mahendra Kabbinahithlu[1], Tobias Lojewski[1], Sergey Kovalenko[2], 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

In nickel oxide (NiO), a correlated transition-metal oxide, the strong electron-electron repulsion splits the d-bands into an occupied lower Hubbard band (LHB) and an unoccupied upper Hubbard band (UHB). The presence of additional oxygen p-bands at the adjacent sites and their interaction with the Hubbard bands leads to complex properties governed by the Hubbard potential (U) and the charge transfer (p ↔ LHB) gap Δ. NiO is a charge-transfer insulator with the p-bands located between the LHB and the UHB ($\Delta < U$). We present excited state dynamics in NiO thin films via time-resolved optical spectroscopy. NiO is pumped above the band gap with 4.8 eV photons and the transient absorption spectrum is probed using a time-delayed supercontinuum. The time-resolved absorption spectrum, shows within the first 500 fs positive pump-induced changes at 2.2 eV and 3.2 eV which are separated from substrate contributions. We also see a strong negative change around 4.3 eV. The positive changes from in-gap states decay on a time scale of 100 fs, while the negative change represents the bleached ground state which recovers within 6 ps, potentially by interaction with phonons.

O 16.3 Mon 15:30 TRE Phy

Photoinduced dynamics of flat bands in the kagome metal CoSn by TR-ARPES — •Denny Puntel[1], Wibke Bronsch[2], Manuel Tuniz[1], Mingu Kang[3], Paul Neves[3], Shiang Fang[3], Efthimios Kaxiras[4,5], Joseph G. Checkelsky[3], Riccardo Comin[3], Fulvio Parmigiani[1,2], and Federico Cilento[2] — [1]Dipartimento di Fisica, Università degli Studi di Trieste, Trieste (Italy) — [2]Elettra - Sincrotrone Trieste S.C.p.A., Trieste (Italy) — [3]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA, USA — [4]Department of Physics, Harvard University, Cambridge, MA, USA — [5]John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA

In kagome systems, the geometry of the lattice localises the electrons in real space, enhancing the correlations and giving rise to flat bands. In CoSn two flat bands with nontrivial topological character lie below the Fermi level [1]. In order to study the response of the localisation mechanism to impulsive excitation, we performed the first time- and angle-resolved photoelectron spectroscopy study on CoSn. At temporal overlap we observe an increase in the electronic temperature, along with a shift and broadening of the flat bands by few meV. A smaller broadening of the flat band persists for the whole duration of the investigated time delay range (about 6 ps). A possible explanation for this broadening is the partial disruption of the real-space electron localisation, because of the increased mobility of the carriers due to the energy injected by the infrared pump pulse.

[1] M. Kang et al., Nat. Commun. 11, 4004 (2020)

Topical Talk O 16.4 Mon 15:45 TRE Phy

Microscopic insight into non-equilibrium dynamics through time-resolved x-ray absorption spectroscopy — •Andrea Eschenlohr — Faculty of Physics and CENIDE, University Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Time-resolved x-ray absorption spectroscopy provides access to element- and chemically sensitive information on the femto- to picosecond timescales of the elementary microscopic processes involving charge, spin and lattice dynamics in solids via optical pump, x-ray probe experiments. Recently implemented specialized x-ray optics at the SCS instrument of European XFEL allow for a simultaneous acquisition of the ground state and optically excited x-ray spectra as well as a reference signal for normalization of the data to the incident x-ray intensity, and thus provide excellent data quality in combination with kHz repetition rates [1]. We employ this scheme to analyze the temporal evolution of the electronic structure of ferromagnetic Ni after optical excitation and distinguish transient broadening and energy shifts in the absorption spectra, which we show to be caused by electron repopulation and correlation-induced modifications of the electronic structure, respectively. Crucially, an ab initio theoretical description requires taking the local Coulomb interaction into account, revealing the temporal interplay between electron correlations and ultrafast spin-dependent charge dynamics [2].

[1] L. Le Guyader et al., arxiv.org/abs/2211.04265

[2] T. Lojewski et al., arxiv.org/abs/2210.13162

O 16.5 Mon 16:15 TRE Phy

Direct observation of light-induced ultrafast currents in black phosphorus — •Maciej Dendzik[1,2], Andrea Marini[3], Samuel Beaulieu[2], Shuo Dong[2], Tommaso Pincelli[2], Julian Maklar[2], R. Patrick Xian[2], Enrico Perfetto[3,4], Martin Wolf[2], Gianluca Stefanucci[4,5], Ralph Ernstorfer[2], and Laurenz Rettig[2] — [1]KTH Royal Institute of Technology, Stockholm, Sweden — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [3]CNR-ISM, Rome, Italy — [4]Tor Vergata University of Rome, Rome, Italy — [5]INFN, Rome, Italy

Understanding intricate details of light-matter interaction on the femtosecond timescale is at the heart of modern photonics and optoelectronics. However, fundamental coupling between charge carriers response and corresponding induced electromagnetic fields upon an ultrafast optical excitation remain largely unexplored in many quantum materials. Here, we present an experimental time- and momentum-resolved photoemission study of black phosphorus (BP) combined with state-of-the-art simulations of ultrafast carrier dynamics and induced fields. We find dramatically different electron dynamics following excitation by light polarized along the zigzag and armchair directions which we associate with a difference in initial population momentum distributions. Remarkably, we observe a sub-picosecond population imbalance of excited carriers with opposite momenta, which correspond to the generation of transient in-plane currents. The results provide a comprehensive picture of the ultrafast carrier dynamics in BP and pave the way for novel applications in optoelectronics or quantum computing.

O 16.6 Mon 16:30 TRE Phy

Band-resolved relaxation of laser-excited gold. — •Tobias Held[1], Pascal D. Ndione[1], Sebastian T. Weber[1], Dirk O. Gericke[2], and Baerbel Rethfeld[1] — [1]RPTU, Kaiserslautern, Germany — [2]CFSA, University of Warwick, Coventry, UK

Irradiation of gold with visible light may excite d-band electrons into the free sp-electron states. This process increases the energy content of the electron system and induces an occupational nonequilibrium. Since the particle exchange is significantly slower than the energy transfer between the electron subsystems, the nonequilibrium band occupation persists long after a temperature can be well defined. Subsequently, density equilibration and the electron-phonon relaxation need to be considered consistently. In Ref. [1], we have simulated the nonequilibrium band occupation with electron density-resolved rate equations and coupled them with a two-temperature model to include the energy transfer from the electrons to the lattice. The results are sensitive to the electron-phonon coupling parameter applied.

Here, we investigate the electron-phonon coupling strength in more detail. We describe the interaction of the d- and sp-electrons with the lattice by complete Boltzmann collision integrals and show that the extracted electron-phonon coupling parameters strongly depend on the band occupation. Consequently, we incorporate this aspect into the simulation by assigning different temperatures to these bands and couple them separately to the phonons.

[1] Ndione, Weber, Gericke, and Rethfeld. Sci Rep, 12(1), 2022

O 16.7 Mon 16:45 TRE Phy

Multi-directional energy transfer across hybrid plasmonic-excitonic interface — •Tommaso Pincelli[1], Thomas Vasileiadis[1], Shuo Dong[1], Samuel Beaulieu[1], Maciej Dendzik[1], Daniela Zahn[1], Sang-Eun Lee[1], Hélène Seiler[1], Yinpeng Qi[1], Rui Patrick Xian[1], Julian Maklar[1], Emerson Coy[2], Niclas S. Mueller[3], Yu Okamura[3], Stephanie Reich[3], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]NanoBioMedical Centre, Adam Mickiewicz University, Poznan, Poland — [3]Freie Universität Berlin, Berlin, Germany

Hybrid plasmonic devices involve a nanostructured metal supporting localized surface plasmons to amplify light-matter interaction, and a non-plasmonic material to functionalize charge excitations. We combine the use of time and angle-resolved photoemission spectroscopy and femtosecond electron diffraction to investigate charge carrier and phonon dynamics in such a system: epitaxial Au nanoislands on bulk WSe_2. The Au nanostructures show delayed electronic temperature increase and cause a shortening of the Σ-exciton lifetime. Lattice heating is accelerated in WSe_2 and delayed in Au. Our results resolve a multi-directional energy exchange on timescales shorter than the electronic thermalization of the nanometal, driven by a non-linear plasmon-exciton interaction. Non-radiative exciton recombination, electron-phonon coupling, and diffusive charge-transfer determine the subsequent energy backflow.

O 16.8 Mon 17:00 TRE Phy

Electronic hybridization and ultrafast dynamics in Terrylene/WS_2 heterostructure. — •Samuel Palato[1], Boubacar Tanda Bonkano[1], Sergey Kovalenko[1], Michele Guerrini[2], Caterina Cocci[2], and Julia Stähler[1] — [1]Humboldt Universität zu Berlin, DE — [2]Carl von Ossietzky Universität Oldenburg, DE

Hybrid organic-inorganic heterostructures offer the possibility of optoelectronic materials with tailored properties. We report on electronic coupling and charge carrier injection in heterostructures formed of terrylene (T) and monolayer WS_2 investigated using steady-state and femtosecond optical spectroscopy.

Terrylene molecules in solution show a typical Frank-Condon transition to a singlet state with a lifetime of 3.7 ns. TD-DFT calculations indicate a transition dipole moment along the long axis of the molecule. In contrast, the spectrum of the T film is complex and implies strong H-aggregation. We assign the dynamics to thermal reorganization of the molecules in the film, giving rise to changes in the magnitude and sign of charge-transfer coupling.

The response of the T/WS$_2$ hybrid indicates direct hybridization of higher-lying exciton states. Upon excitation of T/WS$_2$, the transient response is similar to that of WS$_2$; it suggests direct injection of charge carriers from the organic to the inorganic layer.

The presence of hybrid states and the evidence of direct injection underlines the potential of hybrid organic-inorganic materials with tailored optoelectronic properties.

O 16.9 Mon 17:15 TRE Phy

Ultrafast electron dynamics at D$_2$O/Na$^+$/Cu(111) interfaces — •Florian Kühne[1], Jayita Patwari[1,2], Ping Zhou[1], Karina Morgenstern[2], and Uwe Bovensiepen[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen — [2]Department of Chemistry and Biochemistry, Ruhr-University Bochum

Ion-solvent interactions and electron transfer across the ion-metal hybrid interfaces are of fundamental interest because of their widespread application in energy storage and energy conversion. We aim to understand the effect of solvation on the elementary processes involved in electrochemical applications by developing a microscopic insight into the hybrid interfaces in presence of a solvent. Electron transfer across such interfaces and the consequent relaxation dynamics are the key microscopic steps behind all these applications which occur on femtosecond time scales. Thus, to experimentally analyze the underlying elementary dynamics, we use femtosecond time-resolved two-photon photoelectron spectroscopy (*tr*-2PPE). We discuss the influence of the solvent at the D$_2$O/Na$^+$/Cu(111) interface. We conclude on the local structure - dynamics relation as a function of D$_2$O coverage from the measured energy transfer rate determined by the transient energy shift of the Na 3s resonance on Cu(111). We analyze furthermore the screening of the excited electron in this resonance by the solvent based on the relaxation time variation with D$_2$O coverage.

Funding by the DFG through Project No. 278162697 - SFB1242 and EXC 2033 - 390677874 - RESOLV are gratefully acknowledged.

O 17: Focus Session: Frontiers of Electronic-Structure Theory II (joint session O/HL)

Time: Monday 15:00–17:15 Location: TRE Ma

Topical Talk O 17.1 Mon 15:00 TRE Ma

Coupled-cluster theory for complex solids made ready — •Andreas Grüneis — TU Wien, Institute for Theoretical Physics, Wiedner Hauptstraße 8-10/136, 1040 Vienna, Austria

This talk will review recent progress in applying periodic coupled-cluster theory, which has the potential to achieve a systematically improvable level of accuracy, to solids and surfaces. We will discuss novel techniques that reduce the computational cost by accelerating the convergence of calculated properties towards the complete basis set as well as the thermodynamic limit. The newly developed techniques have been implemented in the free and open source simulation software Cc4s that is interfaced to a growing number of widely-used electronic structure theory codes. These developments have enabled an increasing number of ab initio studies and allowed for assessing the level of accuracy of coupled-cluster theory by comparing to experimental findings as well as quantum Monte Carlo results. The presented applications will cover a wide range of materials science problems including the study of phase diagrams, molecule-surface interactions and properties of defects.

O 17.2 Mon 15:30 TRE Ma

Speedup of structural optimisations using hybrid functionals: Case studies for energy materials — •Daniel Fritsch — Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, Berlin, 14109, Germany

First-principles calculations based on density functional theory have been established as de facto standard for computational materials investigations. Depending on the size of the unit cell, for every material of interest a suitable choice for the unknown exchange and correlation functional has to be made; taking not only into account the desired accuracy, but also the available computational resources.

In recent years, a promising combination of two approaches emerged, starting from a structural relaxation based on a simpler (semi)local functional, supplemented by a single shot hybrid functional calculation. Here, we propose a new method for combining different levels of exchange and correlation functional for structural relaxations.

In a first benchmarking step, this new method will be applied to various sets of promising energy materials, where full hybrid functional calculations are available, with a main focus on the performance of this new approach on the structural properties and the required computational resources. In a second step, this new approach will be applied to materials, which up-to-now have not been accessible to hybrid functional calculations due to the required computational resources. All the presented results on the structural, electronic, and optical properties will be critically discussed alongside experimental findings.

O 17.3 Mon 15:45 TRE Ma

All-Electron Large-Scale Hybrid Density Functional Simulations — Florian Merz[1], Andreas Marek[2], •Sebastian Kokott[3], Christian Carbogno[3], Yi Yao[3], Mariana Rossi[4], Markus Rampp[2], Matthias Scheffler[3], and Volker Blum[5] — [1]Lenovo HPC Innovation Center, Stuttgart — [2]Max Planck Computing and Data Facility, Garching — [3]The NOMAD Laboratory at the FHI-MPG and IRIS-Adlershof HU, Berlin — [4]MPI for the Structure and Dynamics of Matter, Hamburg — [5]Duke University, North Carolina, USA

The localized resolution-of-identity approach [1] enables $O(N)$ hybrid density functional simulations and, thus, the computation of accurate electronic properties of large scale atomistic models in the range of ten thousands of atoms in *FHI-aims* [2]. In this range, parallelization and memory requirements of the exact exchange part, and the evaluation of the Hartree potential remain challenging. The solution of the generalized eigenvalue problem with direct eigensolvers like ELPA [3] naturally becomes a bottleneck due to $O(N^3)$ scaling. In this work, we present recent algorithmic advances for the exact exchange part and the evaluation of the Hartree potential, as well as optimizations of the ELPA library. We systematically perform benchmark tests on CPU and GPU-accelerated architectures covering inorganic solids, large molecules, and organic crystals with up to 50,000 atoms.

[1] Ihrig *et al.*, *New J. Phys.* **17**, (2015).
[2] Levchenko *et al.*, *Comp. Phys. Commun.* **192**, (2015).
[3] Marek *et al.*, *J. Phys. Condens. Matter* **26**, (2014).

15 min. break

O 17.4 Mon 16:15 TRE Ma

A Koopman's compliant exchange correlation potential for semiconductors — •Michael Lorke[1], Peter Deak[2], and Thomas Frauenheim[2] — [1]Institute for Theoretical Physics, University of Bremen, Otto-Hahn-Allee 1, Bremen, 28359, Germany — [2]BCCMS, University of Bremen, Germany

Density functional theory is the workhorse of theoretical materials investigations. Due to the shortcoming of (semi-)local exchange correlation potentials, hybrid functionals have been established for practical calculations to describe surfaces, molecular adsorption, and defects. These functionals operate by mixing between semi-local and Hartree-Fock exchange semi-emprically. However, their parameters have to be optimized for every material separately. To treat materials with a more physics driven approach and without the need of parameter optimization is possible with many-body approaches like GW, but at an immense increase in computational costs and without the access to total energies and hence geometry optimization. We propose a novel exchange correlation potential[1] for semiconductor materials, that is based on physical properties of the underlying microscopic screening. We demonstrate that it reprocuduces the low temperature band gap of several materials. Moreover it respects the required linearity condition of the total energy with the fractional occupation number, as expressed by the generalized Koopman*s theorem. We also show that this novel functional can be used as a kernel in linear response TDDFT to reproduce excitonic effects in optical spectra [1] Physical Review B 102 (23), 235168 (2020)

O 17.5 Mon 16:30 TRE Ma

Accurate and efficient treatment of spin-orbit coupling via second variation employing local orbital basis functions — •Hannah Kleine[1], Andris Gulans[2], Sven Lubeck[1], Cecilia Vona[1], and Claudia Draxl[1] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Department of Physics, University of Latvia

Spin-orbit-coupling (SOC) effects can significantly change the properties of materials containing heavy elements, mostly by introducing shifts and splittings in the band structure. Including SOC effects in density-functional-theory (DFT) calculations can be challenging. In the linearized augmented planewaves plus local orbitals (LAPW+LO) method, SOC is treated as a perturbation and solved by a second variational (SV) scheme where eigenvectors of the scalar-relativistic Kohn-Sham Hamiltonian are used as basis functions for the SO-coupled problem. For certain materials, especially those with strong SOC effects, many SV basis functions are required which leads to high computational costs. By adding LOs to the SV basis, we are able to drastically reduce the basis-set size and thus the computational cost. We implement this approach in the all-electron full-potential computer package exciting [1] and combine it with the use of relativistic LOs to achieve high accuracy results for a variety of different materials.

[1] A. Gulans et al., J. Phys. Condens. Matter 26, 363202 (2014).

O 17.6 Mon 16:45 TRE Ma

Exact sum-rule approach to polarizability and asymptotic van der Waals functionals – derivation of exact benchmarks — •Alberto Ambrosetti[1], John Dobson[2], Matteo Ricci[1], and Pier Luigi Silvestrelli[1] — [1]Dipartimento di Fisica e Astronomia, Università degli Studi di Padova, via Marzolo 8, 35131, Padova, Italy — [2]Nanoscale Science and Technology Centre, Griffith University, Nathan, Queensland 4111, Australia

Using a sum-rule approach we develop an exact theoretical framework for polarizability and asymptotic van der Waals correlation energy functionals of isolated objects[1]. The functionals require only monomer groundstate properties as input. Functional evaluation proceeds via solution of a single position-space differential equation, without the usual summations over excited states or frequency integrations. Explicit functional forms are reported for reference physical systems, including atomic hydrogen and single electrons subject to harmonic confinement, and immersed in a spherical-well potential. Direct comparison with the popular Vydrov-van Voorhis density functional shows that this performs best when density decay occurs at atomic scales. The adopted sum-rule approach implies general validity of our theory, enabling exact benchmarking of van der Waals density functionals, and direct inspection of the subtle long-range correlation effects that constitute a major challenge for approximate (semi-)local density functionals.

[1] M Ricci, PL Silvestrelli, JF Dobson, A Ambrosetti J. Phys. Chem. Lett. 13, 8298-8304

O 17.7 Mon 17:00 TRE Ma

Interacting electrons and bosons in the doubly screened $\widetilde{GW}$ approximation — •Yaroslav Pavlyukh — Department of Theoretical Physics, Wroclaw University of Science and Technology

In Ref. [1] we built on the Generalized Kadanoff-Baym Ansatz for electrons and bosons to map a broad class of nonequilibrium Green's function theories onto a coupled system of ordinary differential equations with linear time-scaling. Available methods to treat *e*-*e* correlations include *GW* [2], *T*-matrix and Faddeev, while *e*-*b* correlations are described by Ehrenfest and second-order diagrams in the *e*-*b* coupling [3].

In this work we present a substantial advance in the treatment of correlations, requiring no extra computational cost and preserving all conserving properties. Specifically, we include the effects of dynamical screening due to *both* *e*-*e* and *e*-*b* interactions ($\widetilde{GW}$ approximation). The $\widetilde{GW}$ extension opens the door to a wealth of phenomena ranging from carrier relaxation and exciton recombination to molecular charge migration and transfer in optical or plasmonic cavities.

[1] Y. Pavlyukh, E. Perfetto, D. Karlsson, R. van Leeuwen, and G. Stefanucci, Phys. Rev. B **105**, 125134 (2022).

[2] E. Perfetto, Y. Pavlyukh, and G. Stefanucci, Phys. Rev. Lett. **128**, 016801 (2022).

[3] D. Karlsson, R. van Leeuwen, Y. Pavlyukh, E. Perfetto, and G. Stefanucci, Phys. Rev. Lett. **127**, 036402 (2021).

O 18: Poster: 2D Materials I

Time: Monday 18:00–20:00 Location: P2/EG

O 18.1 Mon 18:00 P2/EG

CVD growth of 2D transition metal dichalcogenides for electronics and optoelectronics — •Seung Heon Han[1], Ziyang Gan[1], Emad Najafidehaghani[1], Julian Picker[1], Christof Neumann[1], Uwe Hübner[2], Antony George[1], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena, Germany — [2]Leibniz Institute of Photonic Technology (IPHT), Jena, Germany

Two-dimensional (2D) transition metal dichalcogenides (TMDs) are of great interest for fundamental science and technology due to their exceptional electronic and photonic properties. Chemical vapor deposition (CVD) is a viable method for scalable growth of high-quality monolayer TMDs on various substrates and with tailored properties. Here, we present some of our recent research results on the CVD growth of 2D TMDs including monolayer single-crystal TMDs, atomically sharp TMD1-TMD2 lateral heterostructure, and TMD1-TMD2 lateral heterostructure alloys. Moreover, we demonstrate various exciting applications of these monolayers in field-effect transistors, high-performance photodetectors and memtransistors.

O 18.2 Mon 18:00 P2/EG

Assembly of van der Waals heterostructures with ultraclean surfaces for surface science techniques — Keda Jin[1], Tobias Wichmann[1], Felix Lüpke[1], Tomáš Samuely[2], Oleksander Onufriienko[2], F. Stefan Tautz[1], Markus Ternes[1], and •Jose Martinez-Castro[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Centre of Low Temperature Physics, Faculty of Science, P. J. Safarik University & Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia

Van der Waals heterostructures have become an excellent platform to study emerging physical phenomena that are the result of synergistic proximity effects. Until recently, surface science techniques such as ARPES or STM have been excluded from the study of such heterostructures because of their high sensitivity to surface contamination and the fact that they are sensitive to the top-most layer and thus, not being able to use, boron nitride as the encapsulating layer. Here, we report a novel technique for the assembly of van der Waals heterostructures that do not require encapsulation nor melting of polymers, allowing the study of air-sensitive materials surface. By performing low temperature STM, we demonstrate no surface degradation, achieving atomic resolution as well as detecting a perfectly formed superconducting gap in NbSe2.

O 18.3 Mon 18:00 P2/EG

Chemical vapor deposition of MoSe$_2$-WSe$_2$ lateral heterostructures with atomically sharp one-dimensional interfaces — •Ziyang Gan[1], Dorian Beret[2], Ioannis Paradisanos[2], Hassan Lamsaadi[2], Emad Najafidehaghani[1], Christof Neumann[1], Tibor Lehnert[4], Johannes Biskupek[4], Ute Kaiser[4], Laurent Lombez[2], Jean-Marie Poumirol[3], Bernhard Urbaszek[2,5], Antony George[1], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena, Germany — [2]Université de Toulouse, INSA-CNRS-UPS, Toulouse, France — [3]Université de Toulouse, CEMES-CNRS, Toulouse, France — [4]Ulm University, Central Facility of Electron Microscopy, Ulm, Germany — [5]Technische Universität Darmstadt, IPKM, Darmstadt, Germany

Chemical vapor deposition (CVD) enables the epitaxial growth of transition metal dichalcogenide (TMD) lateral heterostructures with one-dimensional interfaces. The growth is achieved by in situ controlling the precursor partial pressures by a two-step heating protocol. Here we characterize the lateral heterostructures of $MoSe_2$-WSe_2 by optical microscopy, Raman spectroscopy, and photoluminescence spectroscopy. Scanning transmission electron microscopy (STEM) demonstrates the high-quality 1D boundary between $MoSe_2$ and WSe_2 with a width of around 3nm. Furthermore, tip-enhanced photoluminescence (TEPL) enables to demonstrate that the heterojunction acts as an excitonic diode resulting in unidirectional exciton transfer from WSe_2 to $MoSe_2$. npj 2D Mater. Appl. 6 (2022) 84

O 18.4 Mon 18:00 P2/EG

Growth and characterization of transition metal dichalcogenides on Au(111) grown by chemical vapor deposition — •Julian Picker[1], Felix Otto[2], Ziyang Gan[1], Maximilian-Schaal[2], Marco Gruenewald[2], Christof Neumann[1], Antony George[1], Roman Forker[2], Torsten Fritz[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Lessingstraße 10, 07743 Jena, Germany — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Transition metal dichalcogenides (TMDs) are layered two-dimensional (2D) materials which have attracted significant attention in recent years. Especially, the exciting properties of their monolayers such as the strong, direct bandgap photoluminescence make them promising for novel electronic and optoelectronic applications. Here, we demonstrate the *ex-vacuo* growth of different TMD monolayers on Au(111) by chemical vapor deposition (CVD). Afterwards, the samples were analyzed in ultra-high vacuum (UHV) with the help of surface sensitive methods, including (low-temperature) scanning tunneling microscopy and spectroscopy (STM/STS), low-energy electron diffraction (LEED), as well as X-ray and angle-resolved ultraviolet photoelectron spectroscopy (XPS/ARPES). While we confirm the formation of high-quality TMDs, we also accessed the structural and electronic properties of these samples down to the atomic scale. In particular, the focus is on the interaction of the TMDs and Au(111) as Au is the most widely used electrical contact material for TMD devices.

O 18.5 Mon 18:00 P2/EG

Unoccupied electronic states of the CDW material 1T-TiSe$_2$ — •Patrick Geers, Marcel Holtmann, and Markus Donath — Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

We present angle-resolved inverse-photoemission (IPE) measurements of the unoccupied electronic structure of the transition metal dichalcogenide 1T-$TiSe_2$. The spectra along the $\overline{\Gamma}\,\overline{M}$ and $\overline{\Gamma}\,\overline{K}$ high symmetry directions are dominated by the Ti-3d bands with rather flat $E(\mathbf{k}_\parallel)$ dispersion. The two energetically separated subgroups e_g and t_{2g} are clearly resolved in the spectra. We observe two e_g bands as expected, while the spectral features of the t_{2g} group are too broad to identify the three predicted states individually. In addition, an image-potential surface state with its free-electron-like dispersion is observed below the vacuum energy. We compare our experimental $E(\mathbf{k}_\parallel)$ results with a theoretical 3D bandstructure by estimating the $\mathbf{k}_\perp$-component of the electron wavevector within the nearly-free-electron approximation. Furthermore, we observe temperature-dependent changes in our IPE data that are attributed to the charge density wave phase transition. Interestingly, only bands of t_{2g} symmetry show energy shifts, proving the orbital selectivity of bands involved in the phase transition [1].

[1] Watson *et al.*, Phys. Rev. Lett. **122**, 076404 (2019).

O 18.6 Mon 18:00 P2/EG

Electronic structure of benzene on MoS2 — •Jan-Philipp Topmöller and Michael Rohlfing — Institute of solid state theory, 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, which might affect its electronic properties. We investigate benzene as such a molecule because it is a small, prototypical one.

We use DFT (LDA, GGA) and DFT-D3 to determine the most stable adsorption position of benzene on MoS2. Subsequently, we use many body perturbation theory to calculate the electronic structure of the adsorbate system and its individual components (MoS2 and the benzene molecule). For example, we find that the HOMO-LUMO of the benzene molecule decreases from 10.5eV by 2.07eV when considering the screening of the monolayer.

O 18.7 Mon 18:00 P2/EG

Evolution of Band structure in 2D transition metal dichalcogenides alloy $Mo_xW_{1-x}Se_2$ — •Sarath Sasi[1], Laurent Nicolaï[1], Lucie Nedvědová[1], Rostislav Medlín[1], Michal Procházka[1], Marie Netrvalová[1], Sunil Wilfred Dsouza[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

Among two-dimensional (2D) materials that emerged in the research scenario after the discovery of graphene, transition metal dichalcogenides (TMDCs) with the general formula MX_2 (M=Mo, W; X=S, Se, Te) attract huge interest as a potential candidate for electronic and optoelectronic applications. There are many artificial methods to engineer the bandgap and spin-polarized bands, such as chemical doping, external electric field etc. Here we are studying the band structure of $Mo_xW_{1-x}Se_2$ single crystals alloy with various stoichiometric ratio x in comparison with WSe_2. The structural characterisation of samples was analysed using Low energy electron diffraction, Raman Spectroscopy and Scanning Electron Microscopy with Energy Dispersive X-Ray Analysis, X-ray photoemission spectroscopy(XPS). Angle-Resolved Photoemission Spectroscopy (ARPES) was used to investigate the electronic band structure of the samples. We evaluated the band dispersion and observed the bands' splitting at the K point. Thus we are evaluating a potential way for band engineering in TMDCs.

O 18.8 Mon 18:00 P2/EG

Tuning the electronic structure of MoS2: how self-intercalation affects screening, interactions and strain — •Borna Pielic[1,2], Matko Muzevic[3], Dino Novko[2], Jiaqi Cai[1], Alice Bremerich[1], Robin Ohmann[1], Marko Kralj[2], Iva Srut Rakic[2], and Carsten Busse[1] — [1]Department Physik, Universitat Siegen, Siegen, Germany — [2]Institute of Physics, Zagreb, Croatia — [3]Department of Physics, Josip Juraj Strossmayer University of Osijek, Osijek, Croatia

Growth of quasi-freestanding 2D materials on van der Waals (vdW) typed substrates can be accompanied by intercalation in order to modify their intrinsic properties. In this work, we epitaxially grow MoS2 monolayer islands on graphene on Ir(111) using two different procedures: (i) two-step molecular beam epitaxy (MBE) growth which results in S intercalation between graphene and Ir(111), and (ii) single-step MBE growth resulting in Mo intercalation. Scanning tunneling microscopy (STM) measurements reveal significant difference in MoS2 islands morphology, and suggests that S intercalation weakens the interaction in the MoS2/graphene stack, while Mo intercalation strengthens it. More importantly, our scanning tunneling spectroscopy (STS) measurements show notable non-rigid shifts of electronic states. The numerical calculations reveal a strong correlation between substrate screening, strain and binding energy, that are in line with experiment. We suggest that this elegant and non-invasive technique could in general be used for altering vdW, electron-electron and electron-phonon interactions in 2D materials.

O 18.9 Mon 18:00 P2/EG

Designing a symmetry-correct minimal model for *2H*-WSe$_2$ — •Max Xylander[1,2], Philipp Eck[1,2], Simon Moser[2,3], Lukasz Plucinski[4], and Giorgio Sangiovanni[1,2] — [1]ITPA, Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence, ct.qmat — [3]EP4, Universität Würzburg, Germany — [4]PGI-6, Peter Grünberg Institut Jülich, Germany

Transition metal dichalcogenides (TMDCs) have been studied for their structure-dependent valley physics. Due to inversion symmetry breaking in combination with strong SOC originating from the transition metal d-shell, these materials posess momentum-dependent spin splitting. Recently, the interest in TMDCs has been further stimulated by twisted moiré lattices, where the emerging flat bands have been associated to chiral representations in twisted bilayer graphene.

Here we present a study on the chiral wavefunctions in *2H*-WSe_2 based on *ab initio* calculations and minimal modeling. Especially, we will focus on an analysis of the irreducible representations, which allow us to design a minimal d-orbital tight-binding Hamiltonian with SOC and inversion symmetry breaking terms. For the validation of the model, we plan further experimental studies with circularly polarized light angle-resolved photoemission.

O 19: Poster: Ultrafast Electron Dynamics at Surface and Interfaces I

Time: Monday 18:00–20:00 Location: P2/EG

O 19.1 Mon 18:00 P2/EG

ULTRAFAST TRANSPORT AND ENERGY RELAXATION OF HOT ELECTRONS ON TMDC/Au/Fe/MgO(001) INVESTIGATED BY TIME RESOLVED PHOTOELECTRON SPECTROSCOPY — •Florian Kühne[1], Jesumony Jayabalan[1], Ping Zhou[1], Detlef Diesing[2], Stephan Sleziona[1], Marika Schleberger[1], and Uwe Bovensiepen[1] — [1]Faculty of Physics and Center for Nanointegration, University of Duisburg-Essen — [2]Faculty of Chemistry, University of Duisburg-Essen

Optically excited electrons are of particular interest in solid state physics because analysis of their dynamics allows an understanding of the microscopic interactions. Excited charge carriers in metals and semiconductors relax on a femto- to picosecond timescale due to electron-electron and electron-phonon scattering. Using a back-side pump geometry in time-resolved photoelectron spectroscopy (PES), see Kühne *et al.*, PRR **4**, 033239(2022), and Beyazit *et al.*, PRL **125**, 076803(2020), we demonstrated the analysis of hot electron transport through metallic heterostructures Au/Fe/MgO(001). By pumping the Fe side by femtosecond laser pulses, hot electrons are excited in the Fe layer and injected into the Au layer. They subsequently propagate to the surface, where they are probed by PES. This work aims to employ these heterostructures as electrodes for photo-excited electrons which are injected into transition metal dichalcogenides. Thereby we aim at an analysis of scattering and propagation of electrons through 2D material layers discerning local and non-local effects. Funding by the DFG through Project No. 278162697 - SFB1242 is gratefully acknowledged.

O 19.2 Mon 18:00 P2/EG

T-ReX: a facility for time-resolved optical and angle-resolved photoemission spectroscopies — •Wibke Bronsch[1], Denny Puntel[2], Manuel Tuniz[2], Fulvio Parmigiani[1,2], and Federico Cilento[1] — [1]Elettra-Sincrotrone Trieste, Trieste, Italy — [2]Università degli Studi di Trieste, Trieste, Italy

The T-ReX laboratory at FERMI, Elettra-Sincrotrone Trieste, is a user facility for ultrafast table-top time-resolved spectroscopies [1-3]. Our facility comprises a number of time-resolved optical spectroscopy (TR-OS) setups and an endstation for time- and angle-resolved photoemission spectroscopy (tr-ARPES). The latter is connected to diverse table-top laser sources, allowing for probe energies ranging from 6 to 30 eV. In order to show how the complementarity of these setups can be beneficial for gaining more comprehensive insights on a sample system, we will present our recent experiments on the charge-density-wave materials VTe2 and VSe2, shedding light on phonon dynamics and electronic structures of the samples under investigation.

[1] S. Peli et al., J. Electron Spectrosc. Relat. Phenomena 243, 146978 (2020).

[2] R. Cucini et al., Structural Dynamics 7, 014303 (2020).

[3] M. Perlangeli et al., Optics Express 28, 8819 (2020).

O 19.3 Mon 18:00 P2/EG

Excited state photoemission momentum maps from time-dependent density functional theory — •Melvin Hodžić, Christian S. Kern, Andreas Windischbacher, and Peter Puschnig — Institute of Physics, NAWI Graz, University of Graz, Austria

Angle-resolved photoemission spectroscopy is a powerful experimental technique to reveal the electronic structure of thin films and interfaces. In particular, constant binding energy angular distributions, so called momentum maps, have been shown to be related to the Fourier transform of the electron-emitting initial state molecular orbital, thereby bridging experiment and theory in photoemission orbital tomography (POT). The extension of POT to optically excited states has, of late, been demonstrated via a femtosecond pump-probe setup, paving the way for tracing the momentum distribution of electrons on ultrafast time scales. However, linking the measured momentum maps to the spatial structure of the exciton wave functions has yet to be achieved. We propose a simple procedure which involves a coherent sum of the ground-state Kohn-Sham orbitals that construct the exciton wave function. Here, we validate this approach by solving Casida's equation for a series of organic molecules in the gas phase leading to optical absorption spectra and exciton compositions. With the gained information, momentum maps obtained via linear-response TDDFT are cross-checked by directly simulating angle-resolved photoemission spectra within the framework of real-time TDDFT. To this end, we record the flux of the emitted electrons through a detector surface.

O 19.4 Mon 18:00 P2/EG

Ultrafast all-optical manipulation of the charge-density-wave in VTe2 — •Manuel Tuniz[1], Wibke Bronsch[2], Denny Puntel[1], Davide Soranzio[3], Davide Bidoggia[1], Steven Johnson[3], Maria Peressi[1], Fulvio Parmigiani[1,2], and Federico Cilento[2] — [1]Dipartimento di Fisica, Università degli Studi di Trieste, Italy — [2]Elettra - Sincrotrone Trieste S.C.p.A., Italy — [3]Institute for Quantum Electronics, ETH Zurich, 8093 Zurich, Switzerland

By means of broadband time-resolved optical spectroscopy (TR-OS) we investigated the ultrafast reflectivity changes caused by collective and single particle excitations in the charge-density wave (CDW) system VTe2. This material has been recently subject of investigation since the modifications in its electronic structure triggered by the CDW formation are strongly orbital-dependent and may give rise to a topological change in specific bands [1]. In our contribution, we show by means of TR-OS measurements the possibility to optically excite the amplitude mode (AM) of the CDW phase and therefore couple to the CDW condensate [2]. Moreover, through double pump experiments, we show the possibility to control the intensity and the phase of the amplitude mode of the system.

References

[1] Mitsuishi, N. et al. Nat. Commun. 11, 2466 (2020).

[2] Schaefer, H. et al. Phys. Rev. B 89, 045106 (2014).

O 19.5 Mon 18:00 P2/EG

Modification of the ultrafast charge carrier dynamics in a molecule/TMDC heterostructure — •Sebastian Hedwig[1], Matthias Rüb[1], Benito Arnoldi[1], Kai Rossnagel[3,4], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics, University of Kaiserslautern and Research Center OPTIMAS, 67663 Kaiserslautern, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24118 Kiel, Germany — [4]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

Tailoring the properties of layered van der Waals materials is one of the most intriguing challenges in the field of 2D materials. While for transition metal dichalcogenides (TMDCs) this is mainly achieved by the formation of heterostructures with other 2D materials, our approach is to functionalize the properties of TMDCs by the adsorption of molecular films. Here we present our recent fs-time-resolved optical-pump XUV-probe ARPES experiments on a C_{60}/TiSe$_2$ heterostructure. TiSe$_2$ was selected since it can host a charge density wave phase at low sample temperature that can be melted by fs pulses [1]. We find a clear modification of the optically induced phase transition dynamics from the CDW into the semi-metallic phase. This observation is discussed in the light of interactions and the interfacial charge carrier dynamics at the C_{60}/TiSe$_2$ interface.

[1] Rohwer T., et al.; Nature, 471, 490, (2011)

O 19.6 Mon 18:00 P2/EG

Analysis of Nonlocal Correlations in $1T$-TaS$_2$ Driven Out of Equilibrium — •Jesumony Jayabalan[1], Florian K. Diekmann[2], Ping Zhou[1], Kai Rossnagel[2], and Uwe Bovensiepen[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

Driving correlated materials out of equilibrium on ultrafast time scales can provide information about the correlation phenomena and their complex free energy landscapes. Time- and angle-resolved photoemission spectroscopy provided access to the ultrafast dynamics of Doublons [Ligges et al., PRL 120, 166401 (2018)] and concluded on presence of empty and doubly occupied sites at few tens of femtosecond timescales which match calculated spectra with 5% static hole doping. Thus the doublon decay was concluded to be mediated in $1T$-TaS$_2$ by the presence of holes. We propose experiments aimed at a doping dependent relaxation dynamics measurements that would reveal the role of screening and charge excitations on such photo-induced states. Two different approaches will be used for doping: 1) $1T$-TaS$_2$ crystals are grown by Ta substitution to induce a less than half filled band and hole doping and 2) surface doping by adsorption of alkali adsorbates on the cleaved $1T$-TaS$_2$ surface. Such doping depending studies at the timescale of the charge density wave amplitude mode potentially allow to examine the role of strong correlations in the coupled electron-lattice dynamics of $1T$-TaS$_2$ as well as possibilities to control two-dimensional correlated surfaces via photo excitation of the substrate.

O 19.7 Mon 18:00 P2/EG

Disentangling HOMO and LUMO excitation in momentum space by means of time-resolved photoemission orbital tomography — Alexa Adamkiewicz[1], Miriam Raths[2], •Marcel Theilen[1], Monja Stettner[2], Sabine Wenzel[2], Mark Hutter[2], Sergey Soubatch[2], Christian Kumpf[2], Francois C. Bocquet[2], Robert Wallauer[1], F. Stefan Tautz[2], and Ulrich Höfer[1] — [1]Philipps-University Marburg, Germany — [2]Peter Grünberg Institute (PGI-3), Jülich Research Centre, Germany

Time-resolved photoemission orbital tomography allows to trace electron dynamics in momentum space by measuring the angle-resolved photoemission intensity on an ultrafast timescale. For molecule-metal interfaces it proved to be a powerful technique to investigate the population dynamics of molecular states [1]. Here, we find for a well-ordered monolayer of CuPc on Cu(001)-2O a delay-dependent change in the momentum pattern of the molecular LUMO. In addition, we show how the temporal evolution of the momentum distribution can be systematically disentangled from contributions of the projected HOMO by varying the pump photon energy and polarization. By aligning the polarization of the pump pulse along the molecular axis of CuPc molecules, we are able to selectively excite molecules of a specific orientation. The temporal evolution of the excitation and decay from the LUMO can be well described by solving the optical Bloch equations for a three-level system.

[1] R. Wallauer *et al.*, Science 371, 1056-1059 (2021).

O 19.8 Mon 18:00 P2/EG

Spin- and valley-dependent charge carrier dynamics in a WSe$_2$ bulk crystal — •Gregor Zinke[1], Sebastian Hedwig[1], Benito Arnoldi[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

The intriguing spin functionalities of transition metal dichalcogenides such as WSe$_2$ are rooted in the spin- and valley-degrees of freedom. These are responsible for the particular spin-texture of TMDCs as well as the helicity- and valley-dependent light absorption. However, despite the clear understanding of the initial spin-and valley-dependent light-matter interaction, a clear picture of the spin-dependent intra- and intervalley scattering of electrons and holes is still elusive. Here, we focus on the ultrafast carrier dynamics in a bulk crystal of WSe$_2$. Using spin-, time- and angle-resolved photoemission with XUV-radiation, we simultaneously image the temporal evolution of the excited carriers in the conduction band as well as the corresponding hole dynamics within the valence band on a fs timescale. The spin-polarization of the initially excited carriers is controlled by the helicity of the optical excitation. We will show clear changes of the spin-polarization of the excited electrons after intra-band scattering from the K- to the Σ-point, and discuss these results in regards to the influence of electron-electron and electron-phonon scattering for the spin-polarized electron population in the conduction band.

O 19.9 Mon 18:00 P2/EG

Ultrafast dynamics of CT excitons in 2d heterostructures investigated with SHG imaging microscopy — •Marleen Axt, Jonas E. Zimmermann, Gerson Mette, and Ulrich Höfer — Fachbereich Physik, Philipps-Universität Marburg, Germany

The exciton dynamics in vertically stacked TMDC heterostructures can be modified by variation of the twist angle between the two layers. Using time-resolved second hamornic (SH) imaging microscopy we observe the ultrafast formation of charge transfer (CT) excitons in micrometer-sized MoS$_2$/WSe$_2$ heterostructures with different stacking angles. We make use of the strong anisotropy of the nonlinear SH response to selectively probe the carrier dynamics in individual layers of the system. For misaligned layers with a stacking angle of 16° the formation of CT excitons takes place within 85 fs after resonant excitation of the WSe$_2$ A excition. In contrast, an alignment close to 2H stacking (52°) leads to an enhanced electronic coupling between the layers resulting in a much faster CT exciton formation time of only 12 fs. Moreover, different formation and relaxation pathways are identified depending on the pump-photon energy.

O 20: Poster: Spins and Magnetism at Surfaces

Time: Monday 18:00–20:00 Location: P2/EG

O 20.1 Mon 18:00 P2/EG

Aging behavior in a self-induced spin glass — Lorena Niggli, •Julian H. Strik, Anand Kamlapure, Mikhail I. Katsnelson, Daniel Wegner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

Elemental neodymium has been shown to be a so-called self-induced spin glass, which, unlike conventional spin glasses, shows glassy behavior solely from frustrated magnetic interactions and in the absence of disorder [1]. Additionally, in contrast to most conventional spin glasses, neodymium has a disorder to order transition. As the temperature increases it goes from the self-induced spin glass phase to a multi-Q long range ordered phase resulting from competing long-range interactions on different length scales [2]. This disorder to order transition might have profound effects on the metastable states and aging dynamics in the low temperature phase. In this study, we use spin-polarized scanning tunneling microscopy combined with varying external magnetic fields to investigate the aging dynamics in the spin glass phase, and quantify this in terms of the various local spin-spin correlations (Q-states) observed. These observations may have interesting implications on the aging behavior in self-induced spin glasses, which might differ from conventional spin glasses.

[1] U. Kamber et al., *Science* **368** (2020).

[2] B. Verlhac et al., *Nat. Phys.* **18** (2022).

O 20.2 Mon 18:00 P2/EG

Tuning the frequency response of stochastically switching orbital states of Fe and Co atoms on black phosphorus — •Kira Junghans, Hermann Osterhage, Werner M. J. van Weerdenburg, Niels P. E. van Mullekom, Ruben Christianen, Eduardo J. Domínguez Vázquez, Hilbert J. Kappen, and Alexander A. Khajetoorians — Radboud University, Nijmegen, The Netherlands

The concept of the atomic Boltzmann machine (BM) is based on the recently discovered idea of orbital memory [1,2]. Orbital memory is characterised by two stable valency configurations [2,3]. By applying a bias voltage to a scanning tunneling microscopy (STM) tip above a threshold, stochastic switching between the states can be induced. The favorability of the individual states depends strongly on the applied bias voltage.

Unlike coupled spins under exchange, leading to bistability, coupled atoms that exhibit orbital memory show multi-stability in their stochastic dynamics. This multi-well energy landscape serves as a basis for the BM and realizing multiple time scales.

Here, we show that single Fe and Co atoms respond frequency and amplitude dependent to an AC component of the applied bias. In addition, we present how the stochastic behavior of coupled atoms in the multi-well regime respond to a harmonic drive voltage.

[1] B. Kiraly et al., Nat. Nanotechnol. 16, 414 (2021).

[2] B. Kiraly et al., Nat. Commun. 9, 3904 (2018).

[3] B. Kiraly et al., Phys. Rev. Research 4, 33047 (2022).

O 20.3 Mon 18:00 P2/EG

Development of a gate-tunable graphene substrate for spins on surfaces — •Paul Greule[1], Máté Stark[1], Wantong Huang[1], David Collomb[1], Daria Sostina[2], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], and Philip Willke[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology, Karlsruhe, Germany

Single spins on surfaces constitute a promising architecture for future quantum technologies as quantum sensors and possible qubits for quantum information processing. The recent combination of electron spin resonance (ESR) and scanning tunneling microscopy (STM) emerges as a new technique to coherently manipulate spin states on a single atom level [Y. Chen et al., Adv. Mater. 2022, 2107534]. Nevertheless, this architecture does not provide yet any method to continuously tune the coupling between single electron spins. Here, we want to introduce graphene field-effect transistors as a new substrate for ESR-STM on single molecules. Gated graphene devices enable tuning of the charge carrier density of the substrate as already shown by means of scanning tunneling spectroscopy (STS) [Y. Zhang et al., Nature Phys. 5, 722-726 (2009)]. This constitutes a promising way to manipulate the substrate-mediated exchange coupling between single spin centers. We present the development of gated graphene devices for STM using single layer graphene. Moreover, we characterize the samples with in-situ transport measurements and show first topographic and spectroscopic STM measurements.

O 20.4 Mon 18:00 P2/EG

Magnetic phase diagram of a YSR-molecule — •Benjamin A. Verlhac[1], Niels van Mullekom[1], Werner M.J. van Weerdenburg[1], Hermann Osterhage[1], Manuel Steinbrecher[1], Katharina J. Franke[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Fachbereich Physik, Freie Universität Berlin, Germany

Yu-Shiba-Rusinov (YSR) states arise from the exchange coupling between a local spin and a superconductor. However, characterizing this exchange interaction, related to Kondo screening, requires a study in magnetic field to understand its interplay with other energy scales, as well as the role of higher spin degrees of freedom. To date, most studies of YSR states have been limited to bulk superconductors, which easily quench in the presence of modest magnetic fields. Here, using high resolution milliKelvin scanning tunneling microscopy and spectroscopy, we characterize the magnetic phase diagram of a molecule on the surface of a thin film superconductor. We observe non-trivial changes in the YSR excitations in applied magnetic field, that cannot be described by the prototypical spin 1/2 model. These variations occur while the superconducting gap remains robust. We relate the changes to the various properties of the molecule, including the role of multiple channels and magnetic anisotropy. We additionally propose a model to understand the various behaviors in the excitation. These results provide an in-depth and detailed approach to understand the role of high spin systems in the presence of Kondo and YSR states.

O 20.5 Mon 18:00 P2/EG

Electronic Structure of Chromium(II)-Bromide Islands on Niobium Diselenide — •Xianzhe Zeng[1], Haonan Huang[1], Sujoy Karan[1], Klaus Kern[1,2], and Christian 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

Chromium(II) bromide is an inorganic two-dimensional (2D) van der Waals material. With molecular-beam epitaxy (MBE), superconducting islands can be formed after evaporating chromium(II) bromide onto a niobium diselenide substrate. Measurements have been conducted on the islands and at the edge of the islands with low-temperature scanning tunneling microscopy and spectroscopy. At the edge of the islands, a subgap peak could be identified from the dI/dV spectrum, suggesting the existence of an in-gap state. Our discovery is the first observation in the chromium(II) bromide-niobium diselenide heterostructure system, providing an interesting comparison with the reported Majorana zero energy mode at the edge of chromium(III) bromide islands growing on the same substrate.

O 20.6 Mon 18:00 P2/EG

Josephson diode effect due to single magnetic atoms — Martina Trahms[1], Larissa Melischek[2], Jacob F. Steiner[2], •Bharti Mahendru[1], Idan Tamir[1], Nils Bogdanoff[1], Olof Peters[1], Gaël Reecht[1], Clemens B. Winkelmann[3], Felix von Oppen[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [3]Université Grenoble Alpes, CNRS, Institut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

Properties of Cooper-pair tunneling through a Josephson junction can be described by the phase difference between two superconductors. In a current-biased Josephson junction, the phase dynamics can be accessed via switching and retrapping currents. Here, we investigate Josephson junctions formed by a superconducting Pb tip and a Pb surface in a scanning tunneling microscope. While pristine Pb-Pb junctions are hysteretic but symmetric in the biasing direction, we observe asymmetric retrapping currents in the presence of single magnetic atoms placed in the junction. The behavior thus mimics diode properties in the retrapping current. We model the phase dynamics of these junctions by an extended resistively and capacitively shunted Josephson junction (RCSJ). We find the asymmetric retrapping current originates in a non-ohmic dissipative channel due to the particle-hole-symmetry-broken Yu-Shiba-Rusinov (YSR) states. By investigating different magnetic adatoms on different Pb surfaces, we carve out a general relation of asymmetric YSR states and asymmetric retrapping currents.

O 20.7 Mon 18:00 P2/EG

Organometallic sandwich complexes as model spin 1/2 impurities on superconductors — •Adithya Sadanandan[1], Lukas Arnhold[1], Nicolaj Betz[1], Andrea L Sorrentino[2], Giulia Serrano[2], Roberta Sessoli[2], Susanne Baumann[1], and Sebastian Loth[1] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]University of Florence, Department of Chemistry 'Ugo Schiff', INSTM Research Unit, Florence, Italy

Self-assembled layers of organometallic sandwich complexes containing transition metal atoms enable selective control of the spin delocalization and hybridization of the molecules with the electron bath of surfaces [1,2]. We study small self-assembled rafts of [CpTi(cot)] sandwich complexes on epitaxial Pb islands on Si(111). [CpTi(cot)] features a single electron in the d orbitals and long coherence times in solution [2] making it an interesting candidate for molecular qubits and a well-defined spin 1/2 system. Using low temperature scanning tunnelling microscopy (STM) we find weakly bound Yu-Shiba-Rusinov states (YSR) in the superconducting gap and a crossover between Kondo screening and spin excitations when superconductivity is quenched by a magnetic field. The simple level structure of [CpTi(cot)] makes it possible to model this system with an Anderson impurity model [3] and deduce the dynamics of the YSR states.

[1] M. Briganti et al., Nano Lett. 22 8626 (2022).
[2] L. C. Camargo et al., Angew. Chem. Int. Ed. 60 2588 (2021).
[3] H. Huang et al., Commun Phys. 3 199 (2020).

O 20.8 Mon 18:00 P2/EG

Electrospray deposition for STM sample preparation in UHV — •Caroline Hommel, Lukas Spree, Dasom Choi, Luciano Colazzo, and Andreas Heinrich — Center for Quantum Nanoscience, 52 Ewhayeodae-gil, Daehyeon-dong, 03760 Seoul, South Korea

Lanthanide single molecule magnets are promising materials for future spintronics applications, such as ultrahigh density memory devices. Using several methods, we have succeeded in synthesizing different double-decker phthalocyanine complexes (M-Pc$_2$; M = Y, Er, Tb) and depositing them on a metal substrate in ultra-high vacuum (UHV) for scanning tunneling microscopy (STM) analysis. Due to their flat geometry they are very well suited for surface deposition. Based on the very well-known chemical properties of the phthalocyanine ligands, it is possible to functionalize them for various purposes. M-Pc$_2$ form ordered structures on the surface, which could be further enhanced by long chain alkane groups on the phthalocyanine ligands. However, such large organic molecules cannot be sublimated without fragmentation. Using electro spray deposition (ESD), thin films of thermally unstable molecules can be deposited directly in UHV. Various parameters, such as pressure, time, and solvent play a role in this process. The influence of the parameters on the deposition will be investigated for M-Pc$_2$ molecules and their chemical derivatives.

O 20.9 Mon 18:00 P2/EG

Scanning tunneling spectroscopy of a spin-crossover complex on a superconductor — •Marten Treichel[1], Florian Gutzeit[2], Jan Homberg[1], Rainer Herges[2], Richard Berndt[1], and Alexander Weismann[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

A spin-crossover complex based on Ni-porphyrin is studied on superconducting Pb(100) using scanning tunneling spectroscopy at 0.3 K. A pronounced molecule-induced surface faceting is found with molecular chains located at multiple substrate steps. The step orientations deviate from the high-symmetry directions of the substrate and appear to be imposed by molecular interactions. Monatomic substrate steps remain undecorated. Conductance spectra reveal spin-flip excitations with clear spatial variations. The data suggest that neighbor molecules are rotated by 90° with respect to each other. We find that an $S = 1$ quantum spin model with the hard axis tilted away from the surface normal reproduces spectra measured in magnetic fields up to 9 T.

O 20.10 Mon 18:00 P2/EG

Strong exchange interaction between open-shell nanographenes and TbAu2 — •Nicolò Bassi[1], Feifei Xiang[1], Jan Wilhelm[2], Roman Fasel[1], and Pascal Ruffieux[1] — [1]Empa-Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — [2]Institute of Theoretical Physics, University of Regensburg, Regensburg, Germany

Rare-earth intermetallic compounds belong to a family of novel substrates, which is becoming a promising platform to control properties of nanomaterials via specific surface-adsorbates interactions. Different combinations, including GdAu2(1), LaAu2(2) and TbAu2(3),have been so far studied. They are all characterized by a ordered hexagonal superstructure with similar lattice constants. Here, we investigate various open-shell nanographenes on TbAu2 alloy by means of STM and STS combined supported by ab inito simulation. For on surface synthesized 7-AGNRs, we find that the predicted spin properties of the end states are indeed conserved on TbAu2. Here, 7-AGNRs are uncharged and the occupied and unoccupied end states have a spin polarization-induced energy splitting of 1.4 eV. In addition, we investigated phenalenyl, the smallest open-shell molecule with spin S = 1/2, at monolayer coverage. Low bias spectroscopy reveals a splitting of the peak of more than 20 mV, which we assign to the exchange interaction between the molecular spin and Tb atoms of the surface layer. These results open new perspectives for studying different open-shell molecules on a magnetic substrate.1 ACS Nano 4, (2010). 2 Phys. Rev. B 88, 125405 (2013). 3 J. Phys. Chem. Lett. 11, (2020).

O 20.11 Mon 18:00 P2/EG

Observation of in-gap states on 4f-shell magnet-superconductor hybrid system — •Yu Wang, Felix Friedrich, Artem Odobesko, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universitaet Wuerzburg, Am Hubland, D-97074 Würzburg, Germany

Magnetic impurities assembled on s-wave superconductor are the prototypical system for the realization of MZMs at the chain ends. Particularly the magnet-superconductor hybrid system of one-dimensional magnetic chains on superconductors has been well demonstrated theoretically and experimentally. Nowadays, various 3d-shell transition metals (Cr, Mn, Fe, Co, Ni) on clean Nb (110) have been studied [1-3]. Among them, only Mn and Fe chains exhibits benchmarks of topological superconductivity with MZMs at the chain ends. In addition to 3d-shell metals as magnetic impurities, 4f-shell magnetic metals could be another option. Among them, Gd shows the highest potential because it has the highest magnetic moment (s = 7/2) in 4f-shell. In this study, we will show that Gd dimers on Nb (110) behave similar as Fe/Mn with two pairs of in-gap states. It could be possible to realize MZMs on Gd chain ends in the future.

[1] D. Crawford and E. Mascot, arXiv: 2109.06894v1 [cond-mat.supercon], (2021)
[2] L. Schneider *et al.*, Nature Physics **17**, 943 (2021)
[3] A. Odobesko *et al.*, Physical Review B **11**, 99 (2019)

O 21: Poster: Scanning Probe Techniques

Time: Monday 18:00–20:00 Location: P2/EG

O 21.1 Mon 18:00 P2/EG

Shot-noise measurements of single-atom junctions using a scanning tunneling microscope — •Verena Caspari, Idan Tamir, Daniela Rolf, Christian Lotze, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Current passing through small constrictions fluctuates due to the discreteness of charge. Measuring this so-called shot noise in atomic-scale superconducting junctions can provide valuable information, from the quanta of charge transferred in the tunneling process to the correlations of the involved tunneling channels. Here, we use a scanning tunneling microscope equipped with a high-frequency, low-temperature amplifier to measure simultaneously the noise characteristics and the differential conductance of two types of Pb-Pb-junctions having different geometries. The first type is created by deposition and approaching single Pb adatoms, while the second type is established by a break-junction technique. We observe a correlation between the noise pattern and the strength of the Josephson current, independent on the method of junction preparation.

O 21.2 Mon 18:00 P2/EG

A second generation millikelvin scanning tunneling microscope with adiabatic demagnetization refrigeration — Taner Esat[1,2], •Denis Krylov[1], Peter Borgens[1,3,7], Xiaosheng Yang[1,3], Peter Coenen[1,4], Vasily Cherepanov[1,4], Andrea Raccanelli[5,7], F. Stefan Tautz[1,2,3], and Ruslan Temirov[1,6] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, 52425 Jülich, Germany — [3]Experimentalphysik IV A, RWTH Aachen University, 52074 Aachen, Germany — [4]mProbes GmbH, 52428 Jülich, Germany — [5]Cryovac GmbH & Co KG, 53842 Troisdorf, Germany — [6]Faculty of Mathematics and Natural Sciences, Institute of Physics II, University of Cologne, 50937 — [7]Current address: Peter Grünberg Institute (Cryo-Lab), Forschungszentrum Jülich, 52425 Jülich, Germany

We present the design of a second generation ultra-high vacuum scanning tunneling microscope (STM) that uses adiabatic demagnetization of electron magnetic moments for controlling its operating temperature down to 30 mK. A high degree of vibrational decoupling promises an outstanding mechanical stability, demonstrated by the first generation of this instrument. Additionally, high frequency cables were implemented in the design in order to enable electron spin resonance experiments.

References: [1] T. Esat, P. Borgens, X. Yang, P. Coenen, V. Cherepanov, A. Raccanelli, F. S. Tautz, and R. Temirov, Review of Scientific Instruments 92, 063701 (2021).

O 21.3 Mon 18:00 P2/EG

atomic friction on TaS2 over a phase transition — •Yiming Song[1], Dirk Dietzel[1,2], and Andre Schirmeisen[1,2] — [1]Institute of Applied Physics (IAP), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Friction force microscopy experiments were performed on tantalum disulfide (TaS2) surfaces as a function of temperature over the phase transition from nearly commensurate charge density wave (NCDW) phase to commensurate CDW phase. A giant frictional peak at the temperature of 187 K which separates CCDW and NCCDW phases when the sample is cooled down is observed. This behavior was investigated in detail by comparing atomic stick-slip motion of the single asperity AFM tip over phase transition. The hysteresis of the first order structural transformation is revealed in stick-slip behaviors during the heating up procedure as well. Besides, the load and velocity dependence of friction on TaS2 surface in CCDW and NCCDW phases have been revealed.

O 21.4 Mon 18:00 P2/EG

Design of a compact dilution refrigerator integrated in a dry mK UHV STM — •Michael Temmen, Simon Gerber, Michael Meyer, and Wulf Wulfhekel — Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

As energy and helium prices are rising we decided to design a new dry, low temperature Scanning Tunneling Microscope with a compact, low ^{3}He volume dilution refrigerator as the main innovation. Special focus was set on the heat exchanger between the still and the mixing chamber as one of the most crucial parts of the system. Next to the standard solution of a tube-in-tube heat exchanger, a new concept of a heat exchanger consisting of two laser cut metal sheets with deep drawn profiles acting as the channels for the Helium and a plain sheet in the middle as a divider is developed. In order to improve heat transfer while keeping the volume minimal, the surface area is increased by electrodeposition of three dimensional porous silver foam. Comparing this concept with the standard solution, an increase in surface area by a factor of 10 could be achieved with a reduction in ^{3}He volume in the exchanger by a factor of 10. The dilution refrigerator is integrated in a small scale cryostat with a closed helium cycle cooled by a pulse tube with a cooling capacity of 400 mW. The complete dilution refrigerator, cryostat and the STM are home-built.

O 21.5 Mon 18:00 P2/EG

Electromagnetic Field Mapping in Plasmonic Nanostructures using Momentum-Resolved Electron Energy-loss Spectroscopy — •Johannes Schultz[1], Jonas Krehl[1], Giulio Guzzinati[2], and Axel Lubk[1,3] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e. V., Helmholtzstraße 20, 01069 Dresden — [2]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp — [3]Institute of Solid State and Materials Physics, Haeckelstraße 3, 01069 Dresden

Localized surface plasmons (LSPs) are collective oscillations of charge carriers arising at interfaces between media of opposite sign of the dielectric functions. Here, spatial confinement of the LSPs, e.g. in nanoparticles (NPs), may lead to enhanced electromagnetic (e.m.) fields of the LSPs due to resonance. This effect is exploited in several application, e.g., surface enhanced Raman spectroscopy. To characterize the e.m. fields scanning transmission electron microscopy in combination with electron energy loss spectroscopy is a frequently used technique due to its high spectral and spatial resolution. Here, the energy loss of the beam electrons (caused by the electric field component of the LSPs parallel to the beam) is measured at different probe positions. This technique has been generalized to additionally probe in-plane field components by measuring the deflection of the beam electrons from their initial trajectory. To that end spectrally resolved deflection maps (so-called $\omega - q$ maps) are recorded at different probe positions which opens up new capabilities to e.g., probe magnetic field contributions of the LSPs at highest spectral and spatial resolution.

O 21.6 Mon 18:00 P2/EG

SpmImage Tycoon: Organize scanning probe microscopy data — •Alexander Riss — Physics Department E20, Technical University of Munich, D-85748 Garching. Germany

The evolution of the field of scanning probe microscopy (SPM) has been associated with development of instrumental capabilities and methods for data acquisition and analysis. However, much less emphasis has been placed on improving the management and organization of the measured datasets. And while datasets can consist of thousands of images and spectra per project, it is not uncommon for researchers to go through each image or spectrum and manually select the channels of interest for each one — only to repeat the same procedure every time they want to analyze their data again.

Here we present a cross-platform application that is designed for fast and effortless organization and basic editing of scanning probe microscopy images and spectra [1]. The application is released under an open-source license and supports automatic channel-of-interest detection, image editing (such as background corrections and contrast adjustment), keywording, star-ratings, powerful search and filtering (e.g., by keywords, data type, location, scan size), as well as export of the data into a PowerPoint-compatible presentation format.

Such easy-to-use tools can lower the entry barrier for aspiring scientists, boost the efficiency of experienced researchers, and help to create and leverage large SPM datasets for machine learning and artificial intelligence applications.

[1] A. Riss. JOSS 7, 4644 (2022)

O 21.7 Mon 18:00 P2/EG

Electric field control of spin transitions in a dimer system using ESR-STM — •Maneesha Ismail[1], Piotr Kot[2], Janis Siebrecht[1], Haonan Huang[1], and Christan R. Ast[1] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Center for Quantum Nanoscience, Institute for Basic Science, Seoul 03760, Republic of Korea

Since the demonstration of the control of spins on the atomic scale, the technique of ESR-STM has been used extensively to explore the field of spintronics. Here, we present a new approach to ESR-STM which uses the bias voltage as a parameter to tune the energy of the Zeeman transition. We demonstrate electronic control of spin resonance transitions in a single molecule. We could observe a strong dependency of the g-factor and tip-field shift on the electric field. Finally, we demonstrate an avoided crossing in the energy levels of a dimer as a function of bias voltage, which corresponds to an entangled state. This could be an important step towards quantum computations as they rely on entanglement opening a more coherent and easier method of electronic spin control.

O 22: Poster Session: Organic Molecules on Inorganic Substrates I

Time: Monday 18:00–20:00 Location: P2/EG

O 22.1 Mon 18:00 P2/EG

Charge-state lifetimes of single molecules on ultrathin insulating films — •Katharina Kaiser[1,3], Leonard-Alexander Lieske[1], Jascha Repp[2], and Leo Gross[1] — [1]IBM Research - Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland — [2]Department of Physics, University of Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany — [3]Present address: Institut de Physique et de Chimie des Matériaux de Strasbourg, Département Surfaces et Interfaces, 23 Rue du Loess, BP 43, 67034 Strasbourg, France

In scanning tunneling microscopy (STM) experiments of molecules on insulating films, tunneling through molecular resonances goes along with transiently charging the molecule. The transition back to its charge ground state by tunneling through the insulating film crucially determines the charging dynamics of the system and with this is essential for understanding, e.g., excited state formation and luminescence quenching in electroluminescence experiments. The two quantities describing these processes are the average charging and discharging time, the latter being the lifetime of the charged state, and they are accessible in STM: By approaching the tip to the molecule at resonant tunnel conditions up to a regime where charge transport is limited by tunneling through the NaCl film the saturation of the tunnel current, which is a direct measure of the molecule's chargestate lifetime and thus provides a means to study charge and exciton dynamics, can be measured. We report on the chargestate lifetimes of individual molecules adsorbed on NaCl films of different thicknesses on Cu(111) and Au(111), and provide insights into the role of the substrate and the spacer layer.

O 22.2 Mon 18:00 P2/EG

Theoretical Investigation of Tetracen-Adsorption on Cu(111)-Substrate — •Florian Alexander Pfeiffer, Johannes Bilk, and Simone Sanna — Institut for Theoretical Physics, Justus-Liebig-University Gießen, Heinrich-Buff-Ring 16, Gießen, 35392, Hesse, Germany

Due to possible catalytic effects of a substrate, chemical reactions can occur within much smaller timescales on metal surfaces than in solutions. Ullman–coupling of Br–substituents to organic molecules, important to biology, chemistry and medicine, might profit of such catalytic effects. Little is known about this reaction on metallic substrates. Theoretical modelling is crucial for understanding the underlying processes. A first step towards such investigation is the first–principle modelling of tetracene–adsorption on Cu(111). Calculation of adsorption geometry and energy as well as charge transfer between molecule and surface is done utilizing density functional theory (DFT). Our calculations show that dispersion forces (van der Waals corrections) need to be taken into account for adsorption modelling. Adsorption energy and geometry as well as charge transfer suggest physisorption of tetracen at Cu(111). The Tersoff–Hamann–approximation allows for simulating STM–images using the DFT–calculated charge density. The STM–images show p_z orbitals of the benzene rings.

O 22.3 Mon 18:00 P2/EG

Effects of oxygen functionalization on the molecule-substrate coupling — •Jonas Brandhoff, Felix Otto, Maximilian

Schaal, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

5,7,12,14-Pentacenetetrone (P4O) is a polycyclic aromatic hydrocarbon which shows promising electronic properties for batteries. Unlike pentacene the π-system is not delocalized over the entire molecule. P4O shows a strong interaction with metal substrates up to a point where the π-system delocalization reemerges partially over the entire molecule. To understand this phenomenon of metallic organic bonding and charge-transfer, as well as the needed interaction strength for enabling a delocalized π-system over the entire molecule, different substrate-P4O systems were investigated. On the one hand, Cu(111) was chosen as a metallic substrate which shows a strong interaction and charge-transfer. On the other hand, the semi-metallic substrate of epitaxial graphene (EG) on SiC(0001) was selected, showing no charge transfer. As an intermediate system, Pt(111) as a noble metal was investigated. Furthermore hexagonal boron-nitride (h-BN) was used to decouple P4O from the Pt(111) substrate. The change in the structure of the adsorbate film was analyzed using STM and LEED. XPS and UPS measurements gain further insights into the electronic properties. Photoemission orbital tomography (POT) was used to characterize the energetic positions of the frontier orbitals.

O 22.4 Mon 18:00 P2/EG

Vectorial Electron Spin Filtering by an All-Chiral Metal-Molecule Heterostructure — •Chetana Badala Viswanatha[1], Johannes Stöckl[1], Benito Arnoldi[1], Sebastian Becker[1,2], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,3] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Department of Chemistry, University of Kaiserslautern, Erwin-Schrödinger-Straße 52, 67663 Kaiserslautern, Germany — [3]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

Chiral-induced spin selective transmission (CISS) has predominantly been explored in structurally helical molecules on surfaces, where the spin selectivity only affects the spin polarization of the electrons along their direction of propagation. Here, we demonstrate[1] a spin-selective electron transmission for a point-chiral molecule 3-Methylcyclohexanone (3-MCHO) adsorbed on the chiral Cu(643) surface. Using spin- and momentum-resolved photoelectron spectroscopy, we detect a spin-dependent electron transmission through a single layer of 3-MCHO molecules that depends on all three components of the electrons' spin. The findings are attributed to the enantiomer-specific adsorption configuration on the surface. This opens the intriguing opportunity to selectively tune CISS by the enantiospecific molecule-surface interaction in all-chiral heterostructures.

[1] J. Phys. Chem. Lett. 2022, 13, 26, 6244-6249.

O 22.5 Mon 18:00 P2/EG

Electronic properties of bi- and peri-tetracene on Cu(111) studied by density functional theory — •Nina Kainbacher[1], Maren Klein[2,3], John B. Bauer[3], Holger Bettinger[3], Heiko Peisert[2], and Peter Puschnig[1] — [1]Institute of Physics, NAWI Graz, University of Graz, Austria — [2]Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany — [3]Institute of Organic Chemistry, University of Tübingen, Germany

Zigzag edged nanographenes with two rows of fused linear acenes, called n-periacenes, have gained increasing attention in the area of organic electronics due to their interesting electronic properties. However, the synthesis is challenging because of their chemical instability. Here we show that a well-ordered monolayer of peritetracene, an n-periacene with four benzene rings in a row, can be produced by depositing the precursor 1,1'-bitetracene on Cu(111) and a subsequent heat treatment. The as-deposited and the annealed films are investigated by STM and UPS and by electronic structure calculations within DFT using a repeated slab approach. We determine the optimal adsorption sites by using damped molecular dynamics and empirical dispersion corrections according to Grimme. We then analyze the electronic structure of the organic/metal interfaces, in particular we focus on the (local) density of states and charge rearrangements upon interface formation which is decisive for the energy level alignment and work function changes. Our results clarify that the interaction of peritetracene with the Cu(111) substrate leads to a charge transfer into the LUMO which is consistent with the experimental observations.

O 22.6 Mon 18:00 P2/EG

Decoupling of vanadyl-naphthalocyanine from a metal substrate by monolayer MoS_2 — •J. Rika Simon, Gaël Reecht, Christian Lotze, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Germany

Phthalocyanines with metal centres are well known for their relative stability on surfaces and are of interest because of the spin they can carry in their metal centres. On metal surfaces, the molecular electronic states are often hydridised with the metal underneath, making it difficult to observe fine details in the electronic structure and inelastic excitations. Using monolayers of semiconducting transition-metal dichalcogenides (TMDCs) as a decoupling layer on top of metal surfaces is a well-established way to allow access to highly resolved $\mathrm{d}I/\mathrm{d}V$ spectra. Here, we use scanning tunnelling microscopy (STM) to probe the properties of vanadyl-naphthalocyanine (VONc) on MoS_2/Au(111). We observe VONc with molecular centres appearing with different apparent heights, which can be interpreted as different configurations of the central oxygen atom sitting on top or below the molecular macrocycle, as observed previously on the closely related molecule vanadyl-phthalocyanine (VOPc) [1,2]. Additionally, we see sharp molecular states in the semiconducting band gap, which are affected by the perturbation potential of the tip [3], causing them to shift in energy across the VONc molecules.

[1] L. Malavolti et al., Nano Lett. 18, 7955 – 7961 (2018)
[2] K. Kaiser et al., ACS Nano 13, 6947 – 6954 (2019)
[3] N. Krane et al., PRB 100, 035410 (2019)

O 22.7 Mon 18:00 P2/EG

Electronic properties of organic/transition metal dichalcogenide heterostructures — •Hibiki Orio[1,2], Maximilian Ünzelmann[1,2], Kiana Baumgärtner[1,2], Christian Metzger[1,2], Markus Scholz[3], Kai Rossnagel[3,4], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Würzburg Dresden, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [4]KiNSIS, Universität Kiel, Kiel, Germany

Adsorption of organic molecules on transition metal dichalcogenides (TMDCs) can modify the electronic properties of both the organic layer as well as the substrate [1]. Here, we investigate the electronic structure of copper phthalocyanine (CuPc) grown on the TMDC TiSe2 using angle-resolved and X-ray photoelectron spectroscopy. We find that the binding energy of the highest occupied molecular orbital increases gradually from 310 to 430 meV upon 4 hours of X-ray radiation. On this poster, we will discuss the origin of this phenomenon.

[1] Y. L. Huang et al., Chem. Soc. Rev., 2018, 47, 3241

O 22.8 Mon 18:00 P2/EG

Ligand Size Controls Surface Chemical Bond: Cobalt Porphyrin versus Cobalt Corrole on the Ag(111) Surface — •Cong Guo, Grigori Pasko, Jan Herritsch, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg

The development of novel functional materials based on biologically relevant molecules such as cobalamins, also referred to as vitamin B_{12}, is an important research topic. In particular, cobalt tetrapyrrole complexes which are related to cobalamins are often-used and well-understood model systems. Due to the structural complexity of the ligands, their interaction and bonding at interfaces is still poorly understood. Using XPS, we compare here a cobalt(II) porphyrin with a related cobalt(III) corrole. The latter exhibits a smaller ring size and acts as a trianionic ligand. In the multilayer, the Co 2p signal of the porphyrin shows the typical appearance of a paramagnetic Co^{2+} center. The corresponding Co 2p signal of the corrole has a similar shape indicating the presence of unpaired electrons in the Co 3d subshell. In the monolayer on Ag(111), both complexes are subject to an interfacial charge transfer from the substrate, as can be seen by the Co 2p signals. Thus, the singly occupied orbitals at the cobalt center are accepting electron density from the substrate. However, the N 1s signal and the valence photoemission spectra indicate that the corrole interacts much stronger with the substrate which is confirmed by periodic DFT calculations. Our study reveals that the two adsorbed complexes differ substantially in their overall interaction with the Ag surface, even though cobalt has a similar electronic state in both cases.

O 22.9 Mon 18:00 P2/EG

Charge Transfer on a 2D Insulator: Influence of the Molecular Functionalzation — •Maximilian Schaal, Jonas Brandhoff, Felix Otto, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg

5, 07743 Jena, Germany

2D materials like hexagonal boron nitride (h-BN) are widely used as interlayer to decouple organic molecules from metallic surfaces. Despite the large band gap of 2D h-BN of $\approx 6\,\mathrm{eV}$, there are also indications for a possible charge transfer into organic molecules. This raises the question: What is the reason for the charge transfer on this 2D insulator?
To address this question, we systematically studied the influence of the molecular functionalization on the lateral structure as well as on the charge transfer on 2D h-BN grown by chemical vapor deposition on Ni(111). Therefore, we compare the structural and electronic properties of pentacene (Pen) monolayers with the oxo-derivatives 6,13-pentacenequinone (P2O) and 5,7,12,14-pentacenetetrone (P4O) by using low energy electron diffraction (LEED), differential reflectance spectroscopy (DRS), X-ray and ultraviolet photoelectron spectroscopy (XPS and UPS) as well as photoemission orbital tomography (POT). For P4O on h-BN/Ni(111) we observed a charge transfer while Pen and P2O remain neutral. This will be discussed in terms of energy-level alignment in these 2D organic/inorganic heterostructures.

O 23: Poster: Surface Reactions

Time: Monday 18:00–20:00 Location: P2/EG

O 23.1 Mon 18:00 P2/EG

XPS Studies of 2-Carbethoxy-3-Phenyl-NBD/QC as MOST Energy Storage System — •Felix Hemauer[1], Valentin Schwaab[1], Eva Marie Freiberger[1], Natalie J. Waleska[1], Andreas Leng[1], Hans-Peter Steinrück[1], and Christian Papp[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Freie Universität Berlin, Germany

Molecular solar thermal (MOST) systems are a candidate for storing solar energy in a chemical manner. The energy-lean norbornadiene (NBD) is converted to its energy-rich valence isomer quadricyclane (QC) in a photoconversion reaction, whereby the energy is stored as strain. Molecular design leads to advantageous light-harvesting properties. In a model catalytic approach, we investigated the surface chemistry of the molecule pair 2-carbethoxy-3-phenyl-NBD/QC on Pt(111), Ni(111) and gold by synchrotron radiation-based XPS. Next to in situ observation of the adsorption, temperature-programmed experiments give insights into thermally induced reactions. Hereby, information on the adsorption behavior, the feasibility of the backward reaction of the QC to the NBD derivative, and the respective stability boundaries on the catalyst surfaces is obtained. On Pt(111), the energy release reaction is found to occur between 140 and 230 K. For Ni(111), the back conversion cannot be triggered thermally; instead, individual decomposition routes are monitored. The gold surface shows the highest catalytic activity with an instantaneous reaction upon adsorption at 110 K. The DFG (Project No. 392607742) supported this work. We thank HZB for allocation of synchrotron radiation beamtime.

O 23.2 Mon 18:00 P2/EG

Multiscale modeling and simulation of texture effects on the corrosion of stainless steel in aqueous media — •Vahid Jamebozorgi[1,2], Karsten Rasim[3], and Christian Schröder[1,2] — [1]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences, 33619 Bielefeld, Germany — [2]Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [3]Miele & Cie. KG, Center for Materials (CFM), Carl-Miele-Straße 29, 33332 Gütersloh

Texture plays a crucial role in physical processes and properties of condensed matter as it is broadly highlighted in the literature. In this work we describe a robust methodology to investigate texture effects which does not suffer from common limitations of quantum based computational approaches in time and space but also can provide the same accuracy as atomistic calculations with orders of magnitude less computational costs. Our methodology is based on the finite element method (FEM) and utilizes 3D digital representations of multi grain microstructures. We demonstrate the efficiency of our approach by studying pitting corrosion in stainless steel. As reflected in literature the irregular geometry of pit expansion through pitting corrosion is mostly caused by texture. We found that the texture significantly affects the pitting corrosion rate and consequently causes various irregular pit growth patterns in granular microstructures. These results are consistent with our DFT and reactive force field molecular dynamics simulations which validate our suggested approach.

O 23.3 Mon 18:00 P2/EG

Model Catalytic Studies on the Thermal Dehydrogenation of 1-Cyclohexylethanol on Pt(111) — •Valentin Schwaab[1], Felix Hemauer[1], Eva Marie Freiberger[1], Natalie J. Waleska[1], Hans-Peter Steinrück[1], and Christian Papp[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Freie Universität Berlin, Germany

The transition to a sustainable, renewable-based energy system requires novel energy storage technologies. So-called liquid organic hydrogen carriers (LOHCs) enable the safe storage of green hydrogen at high volumetric energy densities through the reversible hydrogenation of organic compounds. Particularly interesting systems are secondary alcohols as they often exhibit exceptionally low dehydrogenation temperatures in their reaction to the respective ketone.

Herein, we investigated the thermal dehydrogenation of the LOHC-pair of 1-cyclohexylethanol and acetophenone on a Pt(111) model catalyst. To gain fundamental insight into the reaction behavior and thermal stability limits of the two compounds, temperature-programmed X-ray photoelectron spectroscopy (TP-XPS) experiments were carried out. Based on the obtained C 1s and O 1s data, the dehydrogenation of the alcohol and the formation of potential catalyst poisoning decomposition products are discussed.

We acknowledge financial support by the Bavarian Ministry of Economic Affairs, Regional Development and Energy, and by the DFG (Project No. 419654270). We thank HZB for the allocation of synchrotron radiation beamtime.

O 23.4 Mon 18:00 P2/EG

On-Surface Collision Reactions — Matthew James Timm[1], •Stefan Hecht[2], and Leonhard Grill[1] — [1]Institute of Chemistry, University of Graz, Heinrichstraße 28, 8010 Graz, Austria — [2]Department of Chemistry & IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany

Collisions between atoms and molecules are required to form chemical bonds, and thus lie at the heart of chemistry. Their outcome depends on several parameters: the collision energy, the miss-distance between the centers of the colliding species (the impact parameter), and on the relative alignment of reagents. Studying such reactions on a surface provides a 2D confinement and allows single-molecule imaging by scanning probe microscopy. For surface reactions, it has been demonstrated that the impact parameter can be selected using a 'surface-molecular-beam' of energetic CF2 'projectiles' on a Cu(110) surface [1-2]. The inherent corrugation of Cu(110) collimates the projectiles, allowing them to be aimed at nearby molecular 'targets' at chosen impact parameters. However, the relative alignment of reagents could not be varied until now, due to the singular possible adsorption configurations of the studied targets. Here, a singly-debrominated molecular target has been chosen as it can adopt multiple adsorption alignments relative to the incoming CF2 projectile, thus providing the missing element required for a more general selection of collision geometry. [1] Anggara, K.; Leung, L.; Timm, M. J.; Hu, Z.; Polanyi, J. C.; Sci Adv., 2018, 4, eaau2821. [2] Anggara, K.; Leung, L.; Timm, M. J.; Hu, Z.; Polanyi, J. C.; Faraday Discuss., 2019, 214, 89-103.

O 23.5 Mon 18:00 P2/EG

On-Surface Reaction of Tetraphenylporphyrin with Caesium — •Leonard Neuhaus, Florian Münster, Kassandra Zoltner, Marie Irene Albus, Jan Herritsch, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Tetrapyrroles such as porphyrins and their metal complexes play important roles in living organisms and for various modern technologies. While the surface chemistry of their transition metal complexes has been well studied in the last decades, the complexes of alkali metals are almost completely unknown. Here, we have studied the reaction of tetraphenylporphyrin (H_2TPP) with caesium in the multilayer and monolayer on Ag (111). N 1s X-ray photoelectron spectroscopy (XPS) data indicate complete metalation of the porphyrin in both cases. In complementary temperature-programmed reaction (TPR) experiments performed for the multilayer, the desorbing species were clearly identified by mass spectrometry as Cs_2TPP. DFT calculations indicate that this stable complex has a bipyramidal structure with Cs ions on both sides of the molecular plane.

O 23.6 Mon 18:00 P2/EG

Chemicurrent measurements during oxidation of Mg films with varying impact energy — •Tobias Prost and Hermann Nienhaus — Fakultät für Physik, Universität Duisburg-Essen, Germany

The chemicurrent originating from the oxidation of super thin magnesium films in correlation with the kinetic energies of the impinging particles is investigated. The magnesium layer thickness is kept well below the mean free path in Magnesium (Mg) to reduce the influence of the carrier recombination in the metal film. The I-V characteristics of such Schottky-Diodes show a homogeneous Schottky barrier of 0.68 eV. The reverse current is below 100 pA. Based on the X-Ray photoelectron spectroscopy (XPS) spectra recorded, it can be demonstrated that the magnesium films are not pre-oxidized. A particular focus lays on the determination of the influence of hyperthermic oxygen on the kinetics of the oxidation process. The kinetic energy of the oxygen molecules could be varied between 25 and 300 meV by adding helium. The chemical current measurements with constant kinetic energy confirms the nucleation and growth model. Measurements with different oxygen velocities demonstrate that the reaction efficiency increases with kinetic energy of the molecules.

O 24: Poster: Ion Beam Interaction with Surfaces and Interfaces

Time: Monday 18:00–20:00 Location: P2/EG

O 24.1 Mon 18:00 P2/EG

Defect Engineering of Graphene using Ultra-low energy Ion Implantation — •Felix Junge[1], Manuel Auge[1], Zviadi Zarkua[2], Lino M.C. Pereira[2], and Hans Hofsäss[1] — [1]II. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Quantum Solid State Physics, KU Leuven

Doping and defect engineering of graphene and TMD's to change the electrical properties is highly desirable. To achieve this, we use a unique mass-selected ion beam deposition system, which makes it possible to work in an energy range of $10 < E < 600\,\mathrm{eV}$ for implantation and thus to implant into a 2D-lattice. We use electrostatical masking to control the region which get irradiated. Graphene was doped with Boron and subsequently examined by means of Kelvin probe measurements (SKPM). Furthermore, Helium was implanted into graphene using an electrostatic gradient for decceleration of the ions, to implant the sample with different energies at the same time, which was then analysed with Raman spectroscopy. With these experiments we can see the change of the surface potential of the graphene between a doped and undoped surface region on the one hand and the increasing defect density with increasing implantation energy on the other hand. These results are compared by IMINTDYN (a SDTrimSP based Monte Carlo program for ion implantations) simulations.

Financial support by the DFG and the Volkswagen Foundation is gratefully acknowledged.

O 24.2 Mon 18:00 P2/EG

Sputtering of structured tungsten model surfaces — •Martina Fellinger[1], Christopher Hahn[1], Christian Cupak[1], Gabriele Alberti[2], David Dellasega[2,3], Matteo Passoni[2,3], Matteo Pedroni[3], Andrea Uccello[3], Espedito Vassallo[3], and Friedrich Aumayr[1] — [1]TU Wien, Institute of Applied Physics, Vienna, Austria — [2]Politecnico di Milano, Department of Energy, Milan, Italy — [3]Istituto per la Scienza e Tecnologia dei Plasmi, Consiglio Nazionale delle Ricerche, Milan, Italy

Erosion of first wall materials in nuclear fusion devices limits the lifetime of plasma-facing materials. In the search for materials with low sputtering yields we have investigated not only the sputtering properties of randomly rough [1] but also of oriented and nano-structured tungsten surfaces. Since oriented tungsten nano-columns have shown a favourable reduction in sputtering yield [2], we have now started also to investigate nano-pyramids. These were obtained depositing a tungsten coating on top of chemically etched silicon substrates. The pyramidal surfaces were then exposed to ion irradiation and the subsequent sputtering process was investigated in situ by using a quartz crystal microbalance measurement setup [3]. We will present the experimental results and compare them to state of the art simulations.

[1] C. Cupak et al., Appl Surf Sci 570 (2021)
[2] A. Lopez-Cazalilla et al., Phys Rev Mat 6 (2022)
[3] B. M. Berger et al., Nucl Instrum Methods Phys Res B 406 (2017)

O 24.3 Mon 18:00 P2/EG

In situ GISAXS observation of ion-induced nanoscale pattern formation on crystalline Ge(001) in the reverse epitaxy regime — •Denise Erb[1], Peco Myint[2,3], Kenneth Evans-Lutherodt[4], Karl Ludwig[4,5], and Stefan Facsko[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Division of Materials Science and Engineering, Boston University, USA — [3]X-ray Science Division, Argonne National Laboratory, USA — [4]National Synchrotron Light Source II, Brookhaven National Laboratory, USA — [5]Department of Physics, Boston University, USA

The ion-induced nanoscale pattern formation on a crystalline Ge(001) surface is observed in situ by means of grazing incidence small angle x-ray scattering (GISAXS). Analysis of the GISAXS intensity maps yields the temporal development of geometric parameters characterizing the changing pattern morphology. In comparison with theoretical predictions and with simulations of the patterning process based on a continuum equation we find good agreement for the temporal evolution of the polar facet angle, characteristic length, and surface roughness in the nonlinear regime. To achieve this agreement, we included an additional term in the continuum equation which adjusts the pattern anisotropy.

O 24.4 Mon 18:00 P2/EG

Non-ambient Raman spectroscopy combined with ion bombardment — •André Maas, Lucia Skopinski, Stephan Sleziona, Marika Schleberger, and Lars Breuer — Universität Duisburg-Essen, Fakultät für Physik and CENIDE, Germany

Spectroscopic and electronic characterization of materials under non-ambient condition is an ongoing challenge. Irradiation-induced defects under ambient conditions are usually saturated with adsorbates. The direct analysis of the effects caused by unsaturated defects on the crystal structure and its electronic and optoelectronic properties is however essential to gain a deeper understanding of defect generation, defect saturation and the corresponding relaxations of the lattice due to adsorbates.

A novel experimental setup is presented that allows ion bombardment with two different ion sources and subsequent characterization of samples by a mobile Raman spectrometer in ultra high vacuum. The interaction of highly charged ions (Xe^{17+} - Xe^{40+} at around E_{kin} = 200 keV) from an electron beam ion source (EBIS) can be studied at the University of Duisburg-Essen. A second experimental setup utilizes the swift heavy ions (up to 14.8 MeV/u for $^{238}U^{92+}$) from the CRYRING@ESR at the GSI Helmholtzzentrum für Schwerionenforschung in Darmstadt for defect generation.

Another experiment uses a custom-built cell that allows for electrical and optical characterization of samples under high vacuum and at low temperatures ($\simeq$ 77 K).

O 24.5 Mon 18:00 P2/EG

Ion induced defects in two-dimensional tungsten diselenide boron nitride heterostructure — •Leon Daniel, Stephan Sleziona, Lucia Skopinski, Anke Hierzenberger, Jennifer Schmeink, and Marika Schleberger — Universität Duisburg-Essen, Germany

Monolayer transition metal dichalcogenides (TMDCs) like tungsten diselenide (WSe_2) are highly interesting materials for optoelectronic and valleytronic applications. We used Xe^{q+} ions with E_{kin}=180 keV to deliberately introduce defects into the WSe_2 lattice and compared its optoelectronic properties before and after irradiation with photoluminescence spectroscopy. Encapsulation in hexagonal boron nitride (hBN) isolates the WSe_2 from environmental influences like adsorbates and detrimental interactions with the widely used Si/SiO_2 substrates. We find differences in the photoluminescence response for encapsulated and non-encapsulated WSe_2, which can be explained by the encapsulation preventing saturation of the created vacancies by adsorbates. In particular, there are various localized excitonic states in our different sample systems, and we explain this observation with differing ion interactions with encapsulated and non-encapsulated WSe_2. Furthermore, we observe overall highly increased exciton lifetimes after the irradiation, likely caused by the longer lifetime of the localized excitons.

O 25: Poster: Metal Substrates

Time: Monday 18:00–20:00 Location: P2/EG

O 25.1 Mon 18:00 P2/EG

Ab initio design of Pt-Ir based novel bifunctional electrocatalysts for fuel cell applications — •Halil Ibrahim Sözen[1], Mehtap Oezaslan[2], and Thorsten Klüner[1] — [1]Institute of Chemistry, Carl-von-Ossietzky University of Oldenburg, D-26129 Oldenburg, Germany — [2]Technische Universität Braunschweig, Braunschweig 38106, Germany

Electric vehicles powered by polymer electrolyte membrane fuel cells (PEMFC) have a great potential to reduce a large portion of CO_2 emissions from the transportation sector and facilitate the advent of the hydrogen economy worldwide. However, highly dynamic conditions during the operation of PEMFC in the heavy-duty sector cause hydrogen starvation at the anode electrode, resulting in cell reversal events ($<$ -1.5 V) and therefore carbon oxidation reaction (COR). In this work, we aimed to develop novel bifunctional electrocatalysts for the anode electrode based on Pt-Ir alloys. Our innovative approach involves unifying two functionalities, the hydrogen oxidation reaction (HOR) and oxygen evolution reaction (OER), as an alternative reaction for proton and electron formation to the COR in only one nanoparticle on the same support material. Density functional theory (DFT) based chemisorption energies of H*, O*, OH*, H_2O* and OOH* are reported with the effect of hydroxyl species presence and the effect of pH. Calculated chemisorption energies are implemented to model HOR and OER and plot Gibbs free energy diagrams. Various surfaces such as Pt(111), Pt_3Ir(111), PtIr(111) and Ir(111) have been considered for electrocatalytic reactions and their relative performance is compared.

O 25.2 Mon 18:00 P2/EG

2D Lattice Gas Order-Disorder Transition Observed by LEED and Vibrational Sum Frequency Generation Spectroscopy — •Zhipeng Huang, Tobias Roos, Yujin Tong, and R. Kramer Campen — Faculty of Physics, University of Duisburg-Essen

Order-disorder phase transition of monoatomic superstructures on single crystal surfaces is commonly described by Ising or lattice-gas model. The molecular orientation needs to be considered for modeling the order-disorder transition of diatomic superstructures on single crystal surfaces, but it is challenge to be accessed by experiments.

Here we present our studies on CO ordered overlayers on Pt(111) surface by the surface sensitive thermal desorption spectroscopy (TDS), low-energy electron diffraction (LEED) and polarization dependent sum-frequency generation spectroscopy (SFG). An order-disorder phase transition of CO overlayer is observed by LEED under in-situ heating. The CO stretch vibrational frequency shifts suddenly when the transition happens. Combining LEED superstructure patterns and polarization dependent sum-frequency generation spectroscopy results, we reveal the changes of CO molecular orientation on Pt(111) surface during the order-disorder phase transition. We model the sudden CO stretch frequency shift caused by phase transition and the systematic shift as a function of coverage. These results demonstrate how the CO intermolecular interactions influence the molecular orientation and the stretch vibrational frequency. They provide insights on the change of microscopic potential energy level during the order-disorder phase transition.

O 25.3 Mon 18:00 P2/EG

Formation of solid electrolyte interface from polycaprolactone — •Kazem Zhour[1], Andreas Heuer[1], and Diddo Diddens[2] — [1]WWU Münster, Münster, Germany — [2]Institute Münster (IEK-12) Forschungszentrum Jülich GmbH, Münster, Germany

As for liquid electrolytes, studying the formation of the solid-electrolyte interface and its implications is one of the most important topics in solid-state batteries. In this study, DFT and AIMD calculations were performed to study the decompositions of polycaprolactone, one main constituent of the electrolytes, and its ending groups at the interface. Additionally, the computational lithium electrode method was applied to study the formation of the SEI under external voltage. The AIMD results suggest that the fragments are highly reactive on the Lithium slab where the fragmentation can be observed in less than 1 ps. The decomposition was triggered by the electrons transferred from the slab to the fragments. The electrochemical mechanism shows only slightly weaker energetics with respect to the non-electrochemical one, showing that Li anode readily reacts with the polymer. After the formation of passivation layers (Li2O, LiF or Li2CO3) on top of the anode, the calculations show that only one monolayer protects the molecules from being decomposed at the interface at short interval of time, where the LiF layer seems to have the most robust protection as compared to the other layers. The electrochemical window and the decomposition of the polymer fragments in the presence of a Li cation, TFSI anion, or LiTFSI ion pair without explicit interface have also been also investigated.

O 25.4 Mon 18:00 P2/EG

Single-molecule study of Heck coupling on a Cu(111) surface — •Donato Civita[1], Friedrich Esch[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, Austria — [2]Faculty of Chemistry, TU München, Germany

The interaction of organic molecules with metallic structures is particularly important in heterogeneous catalysis where metallic particles or surfaces help to overcome energy barriers of chemical reactions. This concept is specifically important for Heck cross-coupling, which relies on a palladium catalyst to form a carbon-carbon bond between two different reagents. Model heterogeneous catalysis reactions can be investigated by scanning tunneling microscopy (STM) on metal single crystals. The role of active sites could be determined [1,2], and Heck coupling could be induced thermally [3].

We studied the cross coupling between vinyl-naphthalene (VN) and different halogenated molecules on a Cu(111) surface by STM at low temperatures (7 K). We investigated the bond of the de-halogenated molecules to different atomic structures of the copper surface as well as the thermally induced cross coupling reaction. By the statistical analysis of the products, and STM manipulation of a single metal-organic intermediate we obtain insight into the catalytic activity of the copper surface, and the dependence on the surface morphology.

[1] Hla, S.-W., et al., Phys. Rev. Lett., 85(13) (2000)
[2] Zambelli, T., et al., Science, 273 (1996)
[3] Shi, K.-J., et al., Organic Letters, 19(11) (2017)

O 25.5 Mon 18:00 P2/EG

Cobalt Island Growth on Metallic Surfaces — •Bensu Günay, Christophe Nacci, and Leonhard Grill — University of Graz, Graz, Austria

Molecular-beam epitaxy is an important technique for the fabrication of epitaxial films with reduced dimensionality in the low coverage regime under ultra-high vacuum conditions [1]. Various parameters are important for the morphology of the nanostructures: the flux of the incident atoms, the surface temperature, the source/substrate geometry, and diffusion of the atoms on the surface [2]. In this study, we investigated the growth of cobalt islands on Cu(111) and Au(111) surfaces using different (K-cell and e-beam evaporator) evaporators. The resulting surfaces were then studied by complementary methods: x-ray photoemission spectroscopy (XPS) to analyze the chemical composition of the surface and scanning tunneling microscopy (STM) to investigate the morphology of the islands. The results show how different deposition conditions change the Co growth on the surface.

[1] Prieto, J. E., de La Figuera, J., & Miranda, R. (2000). Surface

energetics in a heteroepitaxial model system: Co/Cu (111). Physical Review B, 62(3), 2126. [2] Negulyaev, N. N., Stepanyuk, V. S., Bruno, P., Diekhöner, L., Wahl, P., & Kern, K. (2008). Bilayer growth of nanoscale Co islands on Cu (111). Physical Review B, 77(12), 125437.

O 26: Poster: New Methods

Time: Monday 18:00–20:00 Location: P2/EG

O 26.1 Mon 18:00 P2/EG

Instrumentation for high-resolution biomolecule imaging enabled by electrospray ion beam deposition (ES-IBD) — •Lukas Eriksson, Tim Esser, Márkó Grabarics, Paul Fremdling, and Stephan Rauschenbach — University of Oxford, Department of Chemistry, United Kingdom

Elucidating the structure of biomolecules is essential to understanding their function. Direct imaging with cryogenic electron microscopy (cryo-EM) or scanning probe microscopy (SPM) is a powerful approach for finding 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 allows for the mass-filtered, soft-landed deposition of a wide mass range of target molecules (m = 100 - 10^6 amu) onto various surfaces, including cryo-EM grids and metal crystals for SPM.[1] This 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.

[1] Paul Fremdling, Tim K. Esser, Bodhisattwa Saha, Alexander A. Makarov, Kyle L. Fort, Maria Reinhardt-Szyba, Joseph Gault, and Stephan Rauschenbach: *A Preparative Mass Spectrometer to Deposit Intact Large Native Protein Complexes.* **ACS nano** 16 (2022)

O 26.2 Mon 18:00 P2/EG

Spectral characterization of battery components from Li-ion battery recycling processes — •Julia Richter[1,2], Sandra Lorenz[2], Christian Röder[1], Roman Tschagaew[1], Yuleika Carolina Madriz Diaz[2], Erik Herrmann[2], Richard Gloaguen[2], and Johannes Heitmann[1] — [1]TU Bergakademie Freiberg, Institute of Applied Physics, Leipziger Str. 23, D-09599 Freiberg (Germany) — [2]Helmholtz-Zentrum Dresden-Rossendorf, Helmholtz Institue Freiberg for Resource Technology, Chemnitzer Str. 40, D-09599 Freiberg (Germany)

The rapid identification of critical compounds in recycling material streams is crucial for an adequate sorting. Recently, the development of adapted multi-sensor systems as well as advanced multi-source data fusion for real-time data integration is in the scope of several research activities. This work deals with the digitalisation of mechanical separation processes in recycling of Li-ion batteries using data which were acquired by hyperspectral sensors. In order to establish a reference data set of the valuable components Al and Cu, in this study a sample set of Al and Cu foils was examined by reflectance spectroscopy in the range (350 * 2500) nm. Based on point measurements and statistical data from imaging sensors, optical material characteristics of the samples were analysed. Proposals for optical sorting steps and possible challenges will be outlined and discussed. This work is financially supported by the Federal Ministry of Education and Research (BMBF) in the framework of the greenBatt cluster within the project DIGISORT.[1] [1] www.greenbatt-cluster.de/de/projekte/digisort/

O 26.3 Mon 18:00 P2/EG

Dynamics of contact electrification — •Andre Mölleken, Hermann Nienhaus, and Rolf Möller — Fakultät für Physik, Universität Duisburg-Essen, Germany

Although the electrical charging of objects brought into contact has been observed for centuries, the details of the underlying mechanism are still not yet fully understood. We have developed an experimental method to follow the charge of a small sphere bouncing on a grounded planar electrode on a time scale down to 1 μs. In case of a contact between two metals, it reveals that the sphere is discharged in the moment of contact, which lasts about 6 to 8 μs. However, at the very moment of disruption of the electrical contact, it regains charge far beyond the expectation according to the contact potential difference. The excess charge rises with increasing contact area.

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

O 26.4 Mon 18:00 P2/EG

Surface tension measurement of pure water in vacuum — •Paul T. P. Ryan, Jiri Pavelec, Jan Balajka, Michael Schmid, and Ulrike Diebold — Institute of Applied Physics, TU Wien, Austria

Very little is known about the surface tension of pure liquids in contact with their pure gaseous phases, i.e. without the presence of other gases or liquid phase contaminants. This is surprising given that contaminants are known to greatly affect surface tensions values[1]. Recently we have developed a method to dose liquid water onto pristine surfaces in UHV using a small cryostat[2]. We combine this approach with the pedant drop method[3] to measure the surface tension of ultra-clean liquids in contact with their pure gaseous phases. In the design, the ultra-clean liquid is condensed onto a small cryostat placed in a vacuum chamber. A pendant drop is formed and carefully photographed allowing the surface tension of the ultra-clean liquid to be directly determined. For these types of measurements accurate knowledge and control of the temperature, pressure and the optics of system is of paramount importance. How these parameters are precisely controlled in the instrument design will be discussed along with initial measurements of ultra-pure water. [1] Yuki Uematsu, et. al., Current Opinion in Electrochemistry, Volume 13, (2019) [2] Jan Balajka, et. al., Science, 361, (2018) [3] Berry, J. D. et. al., J. Coll. Interface Sci. 454, (2015).

O 26.5 Mon 18:00 P2/EG

High-Resolution Imaging of Protein Complexes Enabled by Electrospray Ion-Beam Deposition Sample Preparation — •Asha Thompson, Tim Esser, Markó Grabarics, Isabelle Legge, and Stephan Rauschenbach — University of Oxford, Department of Chemistry, United Kingdom

Structural characterisation of biological molecules such as proteins is essential for insight into their processes and interactions within cells. Samples of mass-filtered molecules adsorbed onto surfaces can be obtained using preparative mass spectrometry techniques such as electrospray ion-beam deposition (ES-IBD). ES-IBD generates intense beams of native proteins which are soft-landed onto surfaces. This produces uncontaminated samples which can be further characterised by transmission electron microscopy (EM) or scanning probe microscopy (SPM).

Here we present the application of this approach for the imaging of proteins showing examples of soluble and of membrane proteins, such as Human C Reactive protein, ferritin, Beta-galactosidase and Aquaporin-Z. We can show that the shape of the protein, its subunit conformation, and stoichiometry are retained, which points to intact secondary structure. [1] We intend to extend this approach to map the interactions of antibodies and their targets in order to provide information about the binding sight, useful for pharmacology.

[1] T. K. Esser, et al, Mass selective and ion-free electron cryomicroscopy protein sample preparation, PNAS nexus, Volume 1, issue 4, 2022

O 26.6 Mon 18:00 P2/EG

RuNNer 2.0: An efficient and modular program for training and evaluating high-dimensional neural network potentials — •Alexander L. M. Knoll[1,2], Marco Eckhoff[3], Jonas A. Finkler[4], Tsz Wai Ko[5], Emir Kocer[1,2], K. Nikolas Lausch[1,2], Moritz R. Schäfer[1,2], Gunnar Schmitz[1,2], Alea Miako Tokita[1,2], and Jörg Behler[1,2] — [1]Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany — [3]ETH Zürich, Laboratorium für Physikalische Chemie, 8093 Zürich, Switzerland — [4]Department of Physics, Universität Basel, 4056 Basel, Switzerland — [5]Department of

NanoEngineering, University of California, San Diego, CA, USA

Machine learning potentials (MLPs) have become a popular tool for large-scale atomistic simulations in chemistry and materials science. They provide efficient access to highly accurate potential energy surfaces (PES) generated from *ab initio* reference calculations. As methods in this field are becoming increasingly complex and reach maturity, the development of efficient and user-friendly tools is also gaining importance. We present the second major release version of RuNNer, an open source, stand alone software package for the construction and evaluation of second, third, and fourth generation high-dimensional neural network potentials (HDNNPs). RuNNer 2.0 unifies an entire workflow in a fully MPI-parallel program: from the generation of atomistic descriptors, over the training of a specific machine learning model, to its final application in molecular dynamics codes.

O 26.7 Mon 18:00 P2/EG

Optical Near-field Electron Microscopy — •Ilia Zykov[1], Hanieh Jafarian[1], Barbara Platzer[1], Thomas Juffmann[1], Amin Moradi[2], Guido Stam[2], Sense Jan van der Molen[2], Ruud Tromp[2], Nestor Fabian Lopez Mora[3], Mariana Manuela Amaro[3], Martin Kalbac[3], Martin Hof[3], and Radek Šachl[3] — [1]University of Vienna, Austria — [2]Leiden University, the Netherlands — [3]J. Heyrovsky Institute of Physical Chemistry, the Czech Republic

Lable- and damage-free imaging of the surface processes on the nanometer scales and over extended periods is required in different fields. Various electron microscopy techniques are applied to meet these requirements. However, the use of electrons in probing the sample may affect some specimens. The novel Optical Near-field Electron Microscopy (ONEM) technique [1] is being developed to overcome this drawback. In the ONEM light nondestructively interacts with a sample. The scattered light from the sample is then transformed into electrons by a nm-thick photocathode layer placed in the near-field region of the sample. The nm resolution images are then achieved through an electron readout using the Low Energy Electron Microscope.

The potential application of ONEM in biochemistry can be to follow the protein dynamics in lipid membranes at single protein resolution. In electrochemistry ONEM will be applied to study the nucleation and growth of nanoscale copper clusters without any electron beam effect.

[1] R. Marchand et al, Phys. Rev. Applied 16, 014008 (2021)

O 26.8 Mon 18:00 P2/EG

Development of a reflektometer for polarised surface sensitive X-ray Absorption Spektroskopy — •Lukas Voss, Frederic Braun, Franz Eckelt und Dirk Lützenkirchen-Hecht — Bergische Universität Wuppertal, Wuppertal, Deautschland

ReflEXAFS measurements represent a powerful tool for surface-sensitive structure investigations. With the help of high-intensity synchrotron radiation on synchrotron beamlines of the third generation, this measurement method can also be used in a time-resolved mode. In order to keep the construction and adjustment time as short as possible, a simple, compact and transportable reflectometer is to be built in order to give other users easy access to this measurement technology. Here we would like to present the current status of the project with the first measurements.

O 27: Overview Talk Katrin Domke

Time: Tuesday 9:30–10:15 Location: TRE Phy

Invited Talk O 27.1 Tue 9:30 TRE Phy

Dive right in! Molecular insights into electrochemical surface science — •Katrin F. Domke — Universität Duisburg-Essen, Germany

Surface scientists have become increasingly aware of the importance of expanding the research focus from classical UHV systems to electrochemical settings that adequately represent realistic working conditions of applications based on solid/liquid reactive interfaces, such as (electro)catalysis or energy conversion schemes. Gathering atomistic understanding about the complex interrelation between charge transfer, chemical conversion and interfacial potential in the present of a solvent is one of the most imminent challenges that surface scientists working with solid/liquid interfaces are facing.

Great efforts are being devoted to the development of novel methodologies to elucidate interfacial electrochemistry mechanisms on the molecular scale. In my talk, I will highlight our advances to achieve simultaneous operando plasmon-supported Raman nanoscopy and break-junction experiments. These approaches allow us to gain unprecedented insights into the correlation of chemical, topographic and electronic properties of individual reactive sites at solid/liquid interfaces, such as catalyst structure or (bio)molecular switches in electrolyte under potential control.

O 28: Organic Molecules on Inorganic Substrates III: Adsorption and Growth I

Time: Tuesday 10:30–13:00 Location: CHE 89

O 28.1 Tue 10:30 CHE 89

Tuning interfaces properties via deposition conditions: thermodynamic's deed and kinetic's contribution — Anna Werkovits, Johannes J. Cartus, Lukas Hörmann, and •Oliver T. Hofmann — Institute of Solid State Physics, Tu Graz

The interface dipole of an inorganic-organic interface depends strongly on the structure, i.e. the polymorph, the organic molecules assume. This is not a subtle effect: In the past years, studies reported work functions differing between up to 3 eV between different polymorphs, illustrating how important it is to control the growth of these interfaces.

In this work, we discuss on the basis of first-principle calcuations how the molecule-substrate, the intermolecular interaction and the size of the molecule affect the relative thermodynamic stability of different phases for different deposition conditions, and how this directly relates to observed work function changes. Based on this, we discuss two ways strategies to tune interface properties. Either, the relative stability can be modified, e.g. by growing the interface in an electric field. Alternatively, it is also possible to exploit kinetic effects during the growth and trap desired phases. Based on the example of TCNE on Cu(111) we discuss how a given phase can be kinetically trapped, and under which circumstances we expect thermodynamic equilibrium to prevail.

O 28.2 Tue 10:45 CHE 89

Homo- and Heterochiral Phases of Quinacridone Monolayers on Ag(110) and Ag(111) — •Ravi Priya, Weishan Wu, Keda Jin, and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, Germany

When adsorbed on a surface, parallel-oriented quinacridone (QA) transforms into a chiral species and lateral interaction between neighboring molecules will depend on the types of enantiomers facing each other. On Ag(111) a homochiral phase comprising rows of (identical) QA has been reported that, upon thermal annealing, converts to a heterochiral phase consisting of alternating pairs (dimers) of the two enantiomers [1]. In our study, we have refined the structural analysis of QA/Ag(111) phases and have extended the available database to QA on Ag(110). Besides SPA-LEED, IR-spectroscopy and TDS were employed to characterize the various phases and associated phase transformations in detail. From IRAS and TDS a stronger molecule-substrate interaction is deduced for Ag(110) as compared to Ag(111). In parallel, interfacial dynamical charge transfer (IDCT) is considerably enhanced for QA/Ag(110) which is ascribed to an extra downshift of the QA-LUMO, increasing its DOS at the fermi energy. Interestingly, IDCT vanishes completely upon the transition of the homochiral to the heterochiral arrangement, both on Ag(111) and Ag(110). This could be explained by a completely empty, or a fully occupied LUMO [2]. As this transition is accompanied by a notable increase in the work

function, we conclude that the latter applies.
[1] https://doi.org/10.1021/jp502148x
[2] https://doi.org/10.1103/PhysRevLett.126.116801

O 28.3 Tue 11:00 CHE 89

Morphology and luminescence of rubrene nanocrystals: a road to tailor nanoplatelets — •Moha Naeimi, Katharina Engster, Christian Völkner, Regina Lange, Sylvia Speller, and Ingo Barke — University of Rostock, Institute of physics, Rostock, Germany

Rubrene ($C_{42}H_{28}$ 5,6,11,12-tetraphenyltetracene) single crystals with a few monolayers had been reported to have high charge mobility of 43 cm^2/Vs [1] and singlet-fission dynamics [2] which are promising properties for the application of excitons for energy transfer or information processing. We aim for the investigation of the spatial distribution of excitons in molecular assemblies on surfaces, requiring thin films or flat nanocrystals. In the present work, we report on the preparation of rubrene platelets by various methods from simple spin-coating to thermal evaporation and broad growth conditions, followed by a high-rate post-annealing temperature treatment on different types of substrates [3]. Ranging from 10 nm to 150 nm, we show that the thickness of rubrene platelets is widely dependent on the rate and time of temperature treatment as well as on the rubrene coverage on the surface. Moreover, we discuss thermal stability and photo-degradation for different morphologies.
[1] A. Saeki. et al., Adv. Mater. 20, 2008, 920-923
[2] Lin Ma. et al., Phys. Chem. Chem. Phys. 14, 2012, 8307-8312
[3] Hyeok Moo Lee. at al., Org. Electron. 12, 2011, 1446-1453

O 28.4 Tue 11:15 CHE 89

Photoelectron Spectroscopy of N-heterocyclic carbenes on Si(111)($\sqrt{3} \times \sqrt{3}$)$R30°$-B surface — •Mike Thomas Nehring[1], Robert Zielinski[1], Mowpriya Das[2], Hazem Aldahhak[3], Conor Hogan[5], Uwe Gerstmann[3], Wolf Gero Schmidt[3], Mario Dähne[1], Martin Franz[1], Frank Glorius[2], and Norbert Esser[4] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Deutschland — [2]Westfälische Wilhelms-Universität Münster, Organisch-Chemisches Institut, Münster, Deutschland — [3]Institut für Theoretische Materialphysik, Universität Paderborn, Paderborn, Deutschland — [4]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Berlin, — [5]Institute for Structure of Matter (ISM-CNR), Rome, Italy

Silicon is the most commonly used element in the industry for manufacturing semiconductor-based components. Semiconductor devices today represent a cornerstone of modern technology, with a multitude of possible applications in research and development. A relatively new area of research is the growth of organic films on modified silicon surfaces. In this work we investigate the adsorption behaviour of various N-heterocyclic carbenes (NHCs) on the Si(111)($\sqrt{3} \times \sqrt{3}$)$R30°$-B surface. This research is conducted using X-ray photonelectron spectroscopy (XPS). By comparison of the experimental spectra with theoretical calculations it is found that all investigated NHCs bind to the Si adatoms of the Si(111)-B surface in an upright adsorption geometry. In addition, the monolayers show a high thermal stability and large work function reductions.

O 28.5 Tue 11:30 CHE 89

Adsorption and thermal stability of phenyl phosphonic acid on cerium oxide: effect of surface morphology, stoichiometry and composition. — •Viacheslav Kalinovych[1], Lesia Piliai[1], Yuliia Kosto[1], Sascha L. Mehl[2], Tomáš Skála[1], Iva Matolinová[1], Vladimír Matolín[1], Kevin C. Prince[2], and Nataliya Tsud[1] — [1]Charles University, Faculty of Mathematics and Physics, Department of Surface and Plasma Science, V Holešovičkách 2, Prague, 18000, Czech Republic — [2]Elettra-Sincrotrone Trieste S.C.p.A., in Area Science Park, Strada Statale 14, km 163.5, Basovizza (Trieste), 34149, Italy

In the present work, the binding properties and thermal stability of the phosphonate group to several well-ordered cerium oxide systems: stoichiometric CeO2(111), fully reduced Ce2O3(111), Ce6WO12(100) and polycrystalline RF CeO2 were studied. Phenyl phosphonic acid (PPA) has been chosen as a molecule consisting of a phosphonate group and a benzene ring. PPA deposition was performed in UHV conditions. The binding properties and thermal stability has been investigated in the range of 25-450 °C by synchrotron radiation photoelectron spectroscopy, resonant photoelectron spectroscopy and near-edge X-ray absorption fine structure spectroscopy. This work comprehensively describes the phosphonate group binding to cerium oxide as a function of substrate morphology, stoichiometry, composition and temperature.

O 28.6 Tue 11:45 CHE 89

Adsorption of a Cyclic (Alkyl)(Amino)Carbene on Si(111)($\sqrt{3} \times \sqrt{3}$)R30°-B: Influence of the Defect Density — •Robert Zielinski[1], Mowpriya Das[2], Canan Kosbab[1], Mike Thomas Nehring[1], Mario Dähne[1], Norbert Esser[1,3], Martin Franz[1], and Frank Glorius[2] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Deutschland — [2]Westfälische Wilhelms-Universität Münster, Organisch-Chemisches Institut, Münster, Deutschland — [3]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Berlin, Germany

N-Heterocyclic carbenes (NHCs) have been shown to be excellent modifiers and anchors for the functionalization of surfaces, but so far mostly on metals. Thus a controlled functionalization of semiconductor surfaces by ordered NHC layers is of great interest. In the present work we investigate the adsorption behavior of cyclohexyl cyclic (alkyl)(amino)carbene (cyCAAC) molecules on the Si(111)($\sqrt{3} \times \sqrt{3}$)R30°-B surface using scanning tunneling microscopy and X-ray photoelectron spectroscopy. We find a self-limited, well-ordered growth of a stable monolayer with large domains characterized by a 3×3 periodicity and an upright adsorption geometry of the molecules. A strong correlation between the domain size and the substrate defect density is found, revealing that the initial molecular adsorption preferentially takes place on a particular type of surface defect. Work function measurements of the cyCAAC monolayer reveal a large reduction of work function.

O 28.7 Tue 12:00 CHE 89

Electronic properties of radical helicene molecules on metallic substrates — •Aleš Cahlík[1], Danyang Liu[1], Carolina A. Marques[1], Ya-Chu Hsieh[2], Yao-Ting Wu[2], Karl-Heinz Ernst[3], and Fabian D. Natterer[1] — [1]Department of Physics, UZH, Zurich, Switzerland — [2]Department of Chemistry, National Cheng Kung University, Tainan, Taiwan — [3]Molecular Surface Science Group, EMPA, Zurich, Switzerland

Helicenes are π-conjugated aromatic compounds with helical shape arising from angularly fused aromatic rings. Radical helicenes combine unpaired electron spins with structural chirality and a π-conjugated framework that can offer intriguing prospects to study the synergy of electronic transport, magnetism and photoactivity. In our work, we employ STM and nc-AFM to investigate an open-shell biradical helicene that we adsorb onto metallic substrates, including magnetic nanoislands. Notably, we observe a Kondo resonance pointing towards the preservation of the open-shell character upon deposition onto Au(111).

O 28.8 Tue 12:15 CHE 89

STM growth studies of 5,14-ol-5,14-diborapentacyclo on low-index coinage metal surfaces — •Wun-Chang Pan[1], Jing Qi[1], Carina Mützel[2], Paula Weber[1], Frank Würthner[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institut für Organische Chemie & Center for Nanosystems Chemistry (CNC), Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

In recent studies [1, 2], heteroatoms-doped precursors have frequently been used to polymerize graphene nanoribbons with a large variety of structures or dopant heteroatoms. Using cryogenic scanning tunneling microscopy, we investigated the structure of self-assembled 5,14-ol-5,14-diborapentacyclo (CM218) on low-index coinage metal surfaces. The main focus of our study is on CM218 on Ag(111), where we find that molecular clusters and chains coexist with molecular islands. At low annealing temperature $T_{\mathrm{ann}} < 100°C$, the islands exhibit a rail track-like structure with a rhomboid-shaped unit cell. Besides, we find irregular clusters and molecular chains. At higher $T_{\mathrm{ann}} \geq 180°C$, islands with a honeycomb (HC) structure are observed. Topographic images of these HCs display a pronounced bias dependence. Molecule-functionalized tips allow for high-resolution images of these structures for which we suggest structural models.
[1] L. Grill and S. Hecht, Nature Chemistry **12**, 115 (2020)
[2] Q. Zhong *et al.*, Nature Chemistry **13**, 1133 (2021)

O 28.9 Tue 12:30 CHE 89

Variable Temperature Scanning Tunneling Microscopy Investigation on Pyrene Monolayers — •Patrick Penner, Xianghui Zhang, Berthold Völkel, and Armin Gölzhäuser — Physik Supramolekularer Systeme und Oberflächen, Universität Bielefeld, Bielefeld, Germany

Pyrene (C16H10) monolayers were prepared by physical vapor deposition on Au(111). Afterwards they were investigated with a variable temperature scanning tunneling microscope with the capability to cool the surface down to -80°C. Without prior cooling, it was impossible to image any molecules at room temperature. After reaching a temperature of 10°C first images could be made. Independent of the temperature the molecules seem to be lying flat on the sample, with a next-neighbor distance of 1.05 nm. After cooling down it was possible to scan at room-temperature small domains of pyrenes near edges of gold terraces, as well as single mobile pyrene molecules.

O 28.10 Tue 12:45 CHE 89

Predicting optimal growth conditions for metastable interface structures — ●Simon Hollweger, Anna Werkovits, Richard K. Berger, Lukas Hörmann, Johannes Cartus, and Oliver T. Hofmann — Institute of Solid State Physics, University of Technology Graz, Austria

For tailoring organic-inorganic interfaces of organic electronic devices controlling the structure that forms during growth is of high importance. Indeed, interface properties often strongly vary for different interface structures. But growing the structure that has the optimal properties for a certain technical application is nothing but trivial, due to the subtle interplay of thermodynamics and kinetics that strongly depend on the growth conditions like temperature and pressure. Therefore, we study how to change temperature and pressure over time in an optimal way to maximize the concentration of a specific high-performance polymorph. The target structure must then be one that is either thermodynamically or kinetically accessible. Finding optimal processing parameters experimentally is a tedious trial and error task, which can be greatly simplified with theoretical guidance. Using the framework of Optimal Control theory, such optimal temperature and pressure protocols can be obtained. In this talk we will demonstrate how this method can be technically implemented, discuss first applications, and point out its possible pitfalls and limitations for the case of designing organic-inorganic interfaces.

O 29: Supported Nanoclusters: Structure, Reactions and Catalysis

Time: Tuesday 10:30–13:00 Location: CHE 91

O 29.1 Tue 10:30 CHE 91

There is life after coking for Ir nanocatalyst superlattices — ●Antonio J Martínez-Galera[1,2], Haojie Guo[3], Mariano D Jiménez-Sánchez[3], Stefano Franchi[4], Kevin C Prince[4], and José M Gómez-Rodríguez[2,3,5] — [1]Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [4]Elettra-Sincrotrone Trieste S.C.p.A., in Area Science Park, 34149 Basovizza (Trieste), Italy — [5]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Achieving superior performance of nanoparticle systems is a major challenge in catalysis. Two main phenomena, occurring during the reactions, hinder the development of the full potential of nanoparticle catalysts: sintering and contamination with carbon containing species, sometimes called coking. Here, we show that Ir nanocrystals, periodically arranged on h-BN supports, can be restored without sintering after contamination by persistent carbon. This restoration yields the complete removal of carbon from the nanocrystals, which keep their crystalline structure, allowing operation without degradation. These findings, together with the possibility of fine tuning the nanocrystals size, confer this nanoparticle system a great potential as a testbed to extract key information about catalysis-mediated oxidation reactions. For the case of the CO oxidation by O2, the existence of chemical processes not observed before in other nanoparticle systems is proven.

O 29.2 Tue 10:45 CHE 91

Formation of the Pd/Co3O4 interface — ●Yaroslava Lykhach[1], Maximilian Kastenmeier[1], Lukáš Fusek[1,2], Matteo Farnesi Camellone[3], Tomáš Skála[2], Nataliya Tsud[2], Viktor Johánek[2], Sascha Mehl[4], Josef Mysliveček[2], Simone Piccinin[3], Olaf Brummel[1], Stefano Fabris[3], and Jörg Libuda[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Charles University, Prague, Czech Republic — [3]Istituto Officina dei Materiali, CNR-IOM, Trieste, Italy — [4]Elettra-Sincrotrone Trieste SCpA, Basovizza-Trieste, Italy

Metal-oxide interfaces play a major role in the design of advanced functional materials for applications in catalysis, energy storage, and nanoelectronics. We investigated the formation of the metal/oxide interface during deposition of Pd nanoparticles onto a well-ordered Co3O4(111) substrate by means of synchrotron radiation photoelectron spectroscopy (SRPES), density functional theory (DFT), and scanning tunnelling microscopy (STM). DFT predicted strong interaction between Pd and Co3O4(111) which resulted in the growth of two-dimensional Pd islands densely covering the substrate. We observed a charge transfer across the metal/oxide interface resulting in partial oxidation of Pd deposits and partial reduction of Co3O4(111). Based on the analysis of the degree of the reduction of Co3O4(111), we found that the charge transfer at the Pd/Co3O4(111) is confined to the near-surface region of Co3O4(111).

O 29.3 Tue 11:00 CHE 91

Structure of PdPt/CeO2/YSZ model systems in operando methane oxidation — ●Jan-Christian Schober[1,2], Silvan Dolling[1,2], Thomas F. Keller[1], and Andreas Stierle[1,2] — [1]DESY, Centre for X-ray and Nanoscience CXNS, Hamburg, Germany — [2]Universität Hamburg, Germany

Due to the high ecological impact of gasoline and diesel fuels, natural gas and biofuel alternatives become more important than ever. Methane is a major component of natural gas and many bio fuels and has a much higher environmental impact than carbon dioxide. Thus, it is vital to ensure the elimination of methane in exhaust gas treatment systems. Pd and PdPt alloy NPs supported by ceria, are among the most active catalysts for the oxidation of methane. Yet, many questions about the interplay of the noble metals with the support, the involvement of palladium oxide species, the role of Pt, and the exact reaction mechanism in the low-temperature regime remain [1,3].

In order to track the active sites and elucidate structure function relationships on an atomistic level we prepare fully epitaxial model systems of PdPt alloy NPs supported by ceria thin films on YSZ single crystals. Using grazing incidence X-ray diffraction techniques in conjunction with our operando catalysis environments we were able to track activity by in-line mass spectrometry and structure of the model catalysts by following the ceria CTRs, as well as Pd, Pt, and their respective oxide Bragg peaks under operando conditions.

[1] J. Dong et al., ACS Catal. 10 (23), pp. 14304-14314.

[2] T. Adriana et al. Surface Science 616, pp. 206-213.

O 29.4 Tue 11:15 CHE 91

Methane activation towards H_2 evolution with subnanometer Ta clusters supported on Pt(111) — ●Tobias Hinke, Kevin Bertrang, Matthias Knechtges, Sebastian Kaiser, and Ueli Heiz — TU Munich, School of Natural Sciences & CRC, Physical Chemistry

The tremendous global energy demand leads to resource shortages as well as environmental consequences. Employing H_2 as an alternative energy carrier from abundant feedstocks such as natural gas is one strategy to tackle these issues. However, efficient hydrogen evolution demands for a fundamental understanding to increase H_2 availability. For this, model systems can be used to elucidate basic principles in chemical reactions, facilitating the design of tailored catalytic systems. Studies of small cationic Ta-clusters and their oxides in the gas phase exhibit high activity towards the activation of highly inert CH_4, yielding Hydrogen, whereas the cluster charge was identified as a key parameter.

These studies are now extended to their supported analogues to approach common catalytic structures. Therefore, Ta_n-clusters ($n < 30$) supported on metal single crystal substrates are investigated under mild conditions in UHV, with regards to their activity towards H_2

evolution from CH_4 via TPD. Characterization was performed via XPS and STM. Supported Ta_8 clusters exhibit size dispersive stability at room temperature and are active towards H_2 evolution form CH_4.

[1] N. Levin et al. *J. Am. Chem. Soc.* **2020**, 142, 12, 5862-5869

O 29.5 Tue 11:30 CHE 91

Ta atoms & clusters on Pt(111) - an XPS study — •Kevin Bertrang, Tobias Hinke, Matthias Knechtges, Federico Loi, Alessandro Baraldi, Sebastian Kaiser, and Ueli Heiz — Physical Chemistry, School of Natural Sciences, & Catalysis Research Center, Technical University of Munich

Thin films comprising Ta/Ta_xO_y have been extensively studied on Pt surfaces. There is still a lack of profound understanding concerning the chemical interaction in the Ta/Pt interface and how it is affected during film growth and oxidation. In particular, an unambiguous attribution of the oxidation state of Ta is lacking which is largely complicated due to the numerous oxides and sub-oxides it can form.

In a bottom up approach we deposited low coverage of Ta atoms & clusters on a Pt(111) surface and probed the system by means of XPS using synchrotron radiation. Oxidation was studied using both atomic and molecular O_2. Stability and surface mobility was studied. At liquid He a high variety of features are observed. In contrast at liquid N_2 most Ta species are mobile and agglomerate to form structures stable up to high temperatures.

O 29.6 Tue 11:45 CHE 91

Cu Nanoparticles on Vicinal and Basal ZnO as Model Catalysts for Methanol Synthesis — •Robert Gleissner[1,2], Simon Chung[1], Esko Erik Beck[1,2], Guilherme D. L. Semione[1,2], Michael Wagstaffe[1], Leon Jacobse[1], Steffen Tober[1,2], Gökhan Gizer[4], Christopher Goodwin[3], Marcus Soldemo[3,6], Mikhail Shipilin[1,3], Patrick Lömker[1,3], Christoph Schlueter[1], Peter Amann[3], Olof Gutowski[1], Ann-Christin Dippel[1], Matthias Muntwiler[5], Vedran Vonk[1], Heshmat Noei[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Universität Hamburg, Germany — [3]University of Stockholm, Sweden — [4]Helmholtz-Zentrum hereon, Gesthaacht, Germany — [5]Paul-Scherrer Institut, Villingen, Switzerland — [6]Stanford University, Stanford, USA

Over recent years, the vicinal ZnO(10-14) surface garnered increased scientific interest, as it combines a high density of surface steps with high stability. However, the role of vicinal ZnO in Cu/ZnO catalysts remained to be investigated. In this study, Cu nanoparticles were grown on vicinal and basal ZnO and studied by STM, LEED, SEM, and ambient pressure XPS, GIXRD, and XRR. On vicinal ZnO, the Cu nanoparticles show a high prevalence of stepped Cu facets, which are interesting for catalytic reactions. Our study elucidates the morphology of the Cu nanoparticles, their interplay with the ZnO support, their stability under oxidation/reduction conditions, and the prospects for improving the activity of Cu/ZnO-based catalysts for methanol synthesis.

O 29.7 Tue 12:00 CHE 91

A hybrid QM/MM framework to study single metal atom adsorption on doped diamond surfaces — •Shayantan Chaudhuri[1], Andrew J. Logsdail[2], and Reinhard J. Maurer[1] — [1]University of Warwick, Coventry, UK — [2]Cardiff University, Cardiff, UK

Polycrystalline boron-doped diamond is widely used as a working electrode material in electrochemistry, and its properties such as a high stability make it an appealing support material for nanostructures for (electro)catalytic applications. Experiments have shown that electrodeposition can lead to the creation of stable small nanoclusters and even single metal adatoms on diamond. We investigate the structural stability and reactivity of single atoms on diamond as predicted by density functional theory. As hybrid functionals are computationally intractable for large-scale periodic surface structures, we use the quantum mechanics/molecular mechanics (QM/MM) methodology to compare different density-functional approximations on equal footing. We investigate the adsorption energy and kinetic stability of metal single atoms on an oxygen-terminated diamond (110) surface and explore the role of structural defects such as vacancies and dopants on metal atom adsorption. Our work forms the foundations for the study of metal nanocluster formation on diamond.

O 29.8 Tue 12:15 CHE 91

Reaction Pathways in Heterogeneous Photoreforming of Tertiary Alcohols — •Martin Tschurl, Clara Aletsee, Paula Neumann, Philip Petzoldt, Carla Courtois, Moritz Eder, and Ueli Heiz — Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

While the oxidation of tertiary alcohols remains a challenge in organic chemistry, heterogeneous photocatalysis opens up new pathways for their conversion. In this contribution, we discuss the selective oxidation of those alcohols under illumination on titania model photocatalysts. We reveal the processes occurring on the surface of a rutile single crystal in studies under ultra-high vacuum conditions and address the role of the pressure gap by comparing those results with reactions of titania powders at ambient pressure. Furthermore, we demonstrate the impact of co-catalyst loading on the selectivity of the reaction and explain the underlying reaction mechanisms.

O 29.9 Tue 12:30 CHE 91

Bottom-up synthesis and transfer of free-standing nanocluster arrays supported by carbon — •Tobias Hartl[1], Stefan Schulte[1], Moritz Will[1], Pantelis Bampoulis[1,2], Rajendra Singh[3], Jani Kotakoski[3], Jan Knudsen[4], and Thomas Michely[1] — [1]Universität zu Köln — [2]MESA+ Institute for Nanotechnology — [3]Universität Wien — [4]MAX IV Laboratory

Cluster superlattices exhibit unique properties stemming from their small size and dimensionality. However, their use in applications is hampered by their low stability when exposed to application relevant conditions, e.g. ambient pressure or high temperature. We succeeded in synthesizing free-standing cluster superlattice membranes (CSLM) which are stable at these conditions. CSLMs consist of a 2D lattice of similar-sized nanoclusters sandwiched between graphene (Gr) and an amorphous carbon (a-C) matrix. In order to make the membrane useful for experiments in nanocatalysis, it needs to be lifted off from the Ir(111) substrate and flipped over, to expose it's Gr bottom side. This enables the removal of the covering Gr sheet and provides access to the clusters in the a-C matrix. Turning the membrane around requires a double transfer process, which is preceded by water and gas intercalation below the membrane. The transfer process consists of a first pick-up with a PDMS stamp, then a second pick-up from the PDMS stamp onto a polycarbonate stamp and finally the transfer to a new substrate. We present the fabrication and transfer processes of the membranes and explore the thermal stability and the physicochemical properties of this novel nanomaterial via XPS, TEM and STM.

O 29.10 Tue 12:45 CHE 91

Changing surface morphology and chemistry by scalable atmospheric pressure plasma treatment — •Timo Wagner[1], Nicolas Wöhrl[1], Vineetha Vinayakumar[2], Doris Segets[2], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Particle Science and Technology (IVG-PST) and CENIDE, University of Duisburg-Essen

Nickel foams provide a large specific surface area. Yet, compared to bulk nickel plates, they are less desirable for industrial applications due to their higher cost and more difficult handling. As part of H2Giga, the hydrogen flagship project by the German Federal Ministry of Education and Research (BMBF), we developed a plasma treatment for industry relevant nickel plates and catalyst particles. In a common manufacturing process for electrolyzers, nickel plates or meshes are first coated with a suspension of catalyst particles. Afterwards the solvents get thermally evaporated, yielding the finished electrode. With our process, the blank nickel surface can be roughened up by exposing it to a nitrogen plasma as a form of pre treatment. Also after coating, an exposure to a nitrogen plasma shows significant morphological changes. The individual particles coalesce to bulbs, that are again interspersed by a sponge-like porous structure. these structures have shown to notably improve the electrochemical performance of the electrodes, decreasing the overpotential by ca. 100mV.

O 30: 2D Materials I: Electronic Structure

Time: Tuesday 10:30–13:15 Location: GER 37

O 30.1 Tue 10:30 GER 37

Controlling the charge density wave transition in single-layer TiTe$_{2x}$Se$_{2(1-x)}$ alloys by band gap engineering — •Tommaso Antonelli, Andela Zivanovic, Chiara Bigi, Brendan Edwards, Akhil Rajan, and Phil King — University of St. Andrews

The narrow gap semiconductor monolayer (ML) TiSe$_2$ undergoes a controversial charge density wave transition [1, 2] whose nature is still poorly understood. Recently, a similar instability has been observed in the sister semimetallic compound ML-TiTe$_2$ showing a weaker CDW coupling as compared to the selenide compound [3, 4]. Using molecular beam epitaxy, we grow ML-TiTe$_{2x}$Se$_{2(1-x)}$ alloys to engineer the band gap in the normal phase and tune the CDW coupling in the system. Performing angle-resolved photoemission spectroscopy on the alloy films, we demonstrate the effective semiconductor to semimetal transition in the high-temperature phase band structure and observe the consequent modulation of the CDW critical temperature. Our experimental results are rationalised using a simple theoretical model bringing new insight on how to manipulate this collective phase at the 2D limit.

[1] P. Chen *et al.*, Nat. Commun. 6, 8943 (2015) [2] M. D. Watson *et al.*, 2D Materials 8, 015004, (2021) [3] P. Chen *et al.*, Nat. Commun., 8, 516 (2017) [4] T. Antonelli *et al.*, npj Quantum Mater. 7, 98 (2022)

O 30.2 Tue 10:45 GER 37

Charge density wave in 2H-NbSe$_2$ studied by combined STM/nc-AFM — •Nikhil Seeja Sivakumar[1], Marion van Midden Mavric[1], Nora Huijgen[1], Umut Kamber[2], Daniel Wegner[1], Alexander Ako Khajetoorians[1], and Nadine Hauptmann[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Department of Physics, Princeton University, USA

Van der Waals materials exhibit interesting quantum phases such as charge density waves (CDW) which originate from an electronic instability along with structural rearrangements. One example is 2H-NbSe$_2$ which exhibits an incommensurate CDW below 33 K. The origin of the CDW in 2H-NbSe$_2$ is currently understood to be driven by electron-phonon coupling [1]. To characterize the CDW with atomic scale resolution, Scanning Tunneling Microscopy (STM) is frequently used which is sensitive to the convolution of the geometric structure and the local density of states.

Here, we utilize combined low-temperature STM and non-contact Atomic Force Microscopy (STM/nc-AFM) based on the qPlus design to study the CDW at the surface of 2H-NbSe$_2$. We detail the distancedependent contrast of the atomic lattice and the CDW in current and frequency shift images. We further compare force spectroscopy data at selected positions of the CDW unit cell and analyze different force contributions.

[1] Flicker, F., van Wezel, J. Nat. Commun. 6, 7034 (2015).

O 30.3 Tue 11:00 GER 37

Circular dichroism in valence band photoemission from CrGeTe$_3$ — •Honey Boban[1], Mohammed Qahosh[1], Xiao Hou[1], Magdalena Szczepanik[2], Ewa Partyka-Jankowska[2], Tomasz Sobol[2], Tom G Saunderson[3,4], Yuriy Mokrousov[3,4], Mathias Kläui[3], Claus Michael Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6, FZ Jülich, Germany — [2]NSRC SOLARIS, Poland — [3]University of Mainz, Germany — [4]PGI-1, FZ Jülich, Germany

CrGeTe$_3$(CGT) is a layered ferromagnetic semiconductor with a bulk Curie temperature (T$_c$) of 63K[1] and an indirect bandgap of 0.4eV[2]. A previous band structure mapping study of CGT[1] revealed band renormalizations below and above T$_c$ and resonance enhancements at the Cr 3p absorption edge. CGT contains large Te atoms (Z=52), therefore spin-momentum locked splittings, Weyl nodes, and anticrossings are expected due to a combination of ferromagnetism and spin-orbit coupling, as well as the related Berry curvature physics. We performed light-polarization-dependent and temperature-dependent angle-resolved photoemission (ARPES) measurements on surfaces of bulk CGT. We have observed renormalizations in the dichroic ARPES maps below and above T$_c$, which could be indirectly related to magnetic ordering, even though our technique most likely averages spin-up and spin-down domains. Circular dichroic ARPES maps contain an intrinsic contribution due to the orbital angular momentum through dipole selection rules and an extrinsic contribution due to the experimental geometry. Our current work focuses on disentangling the two effects. Ref: [1] PRB **101**, 205125(2020), [2] PRB **98**, 125127(2018)

O 30.4 Tue 11:15 GER 37

Investigation of phase-transitions in MoTe$_2$ using ToF-MM — •O. Fedchenko[1], F. Diekmann[2], K. Medjanik[1], M. Kallmayer[3], S. Babenkov[1], D. Vasilyev[1], O. Tkach[1], M. Souliou[4], M. Frachet[4], M. Le Tacon[4], K. Rossnagel[2], A. Winkelmann[5], G. Schönhense[1], and H.-J. Elmers[1] — [1]JGU, Institut für Physik, Mainz, Germany — [2]Institut für Experimentelle und Angewandte Physik, CAU Kiel, Germany — [3]Surface Concept GmbH, Mainz — [4]KIT, IQMT, Karlsruhe, Germany — [5]ACMN, AGH University of Science and Technology, Krakow, Poland

MoTe$_2$ is unique among transition metal dichalcogenides (TMDCs) because it can be grown in both the semiconducting (2H) and semimetallic (1T') phase. The transitions between these phases can be controlled with temperature and doping concentration. Using time-of-flight momentum microscopy (ToF-MM), the thermally-induced inversion symmetry breaking in doped Mo$_{1-x}$W$_x$Te$_2$ is investigated. Pristine MoTe$_2$ and Mo$_{0.98}$W$_{0.02}$Te$_2$ take the 2H phase, which does not show any thermal induced phase transition. For increased W doping concentration we obtain the metastable monoclinic 1T' phase at 300K (RT), which then can be transformed to the orthorhombic T$_d$ phase at T<170 K (LT). Raman and XRD measurements confirm the structural transitions.The T$_d$-phase exhibits topological states identified by Fermi arcs, up to binding energy of E$_B$ = 75 meV.

O 30.5 Tue 11:30 GER 37

Geometry-induced spin-filtering in photoemission maps from WTe$_2$ surface states — Tristan Heider[1], Gustav Bihlmayer[2], Jakub Schusser[3,4], Frierich Reinert[4], Jan Minar[3], Stefan Blügel[2], Claus M. Schneider[1], and •Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum Jülich — [2]PGI-1 Forschungszentrum Jülich — [3]University of West Bohemia, Pilsen, Czech Republic — [4]Experimentelle Physik VII, Universität Würzburg

WTe$_2$ is a semi-metallic quantum material that exhibits non-saturating magnetoresistance and potentially hosts Weyl type-II nodes [1]. Through laser-driven spin-polarized ARPES Fermi surface mapping, we demonstrate highly asymmetric spin textures of electrons photoemitted from the surface states of WTe$_2$ [2]. Such asymmetries are not present in the initial state spin textures, which are bound by time-reversal and crystal lattice mirror plane symmetries. The findings are reproduced qualitatively by theoretical modeling within the one-step model photoemission formalism, and a simple toy-model suggests that a similar effect shall be observed in other materials with low symmetry. Our spin-polarized maps, with detail comparable to the previous spin-integrated maps [3], have been measured using the newly developed high-resolution instrument at PGI-6 in Jülich that is based on a hemispherical analyzer with the scanning lens, an exchange-scattering spin detector, and a *cw* 6 eV laser.

[1] P. K. Das et. al. Electron. Struct. 1, 014003 (2019) and refs. therein. [2] T. Heider et al., arXiv:2210.10870 (2022). [3] F. Y. Bruno et al., Phys. Rev. B 94, 121112 (2016).

O 30.6 Tue 11:45 GER 37

Observing Duffing oscillations in 2D materials by ultrafast electron imaging — •Alexander Schröder, Lina Hansen, and Sascha Schäfer — Institute of Physics, University of Oldenburg, Germany

Two-dimensional materials are an ideal test bed for probing non-linear mechanical resonances. With sample thicknesses down to the atomic scale, the nonlinear regime of mechanical resonances can be observed even for small actuation forces. Previously, the response of such nano- and micromechanical systems was probed by optical or electronic means, leaving details of the mechanical mode structures and their connection to atomic defects unresolved. Here, we present the nanoscale probing of nonlinear Duffing resonances in free-standing graphite membranes using large-angle convergent-beam diffraction in an ultrafast transmission electron microscope equipped with an event-based electron detector with nanosecond temporal resolution. The vibrational membrane modes are excited by a diode laser beam with a tunable modulation rate and a series of resonances are observed in the MHz frequency range with high quality factors (up to 10^4). As expected for prototypical Duffing resonances, increasing the optical excitation strength yields a strong nonlinear hardening of the oscillator, with an increase in vibrational amplitude, an asymmetric broadening of the resonance line shape, bistable behavior, and a characteristic frequency-dependent phase shift. The novel detection scheme as proposed here is ideally suited for characterizing the behavior of ultra-small resonators difficult to address with other techniques.

O 30.7 Tue 12:00 GER 37

Limitations of supercell extrapolation for charged defects at surfaces & 2D materials — •Christoph Freysoldt[1], Anne Marie Z. Tan[2,3], Richard G. Hennig[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Department of Materials Science and Engineering, University of Florida, Gainesville, Florida 32611, USA — [3]School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore 639798, Singapore

Ab initio calculations of defects often employ the repeated slab approach for its simplicity. Unfortunately, spurious interactions between the defect and its periodic images make it sometimes challenging to estimate the dilute limit, that is relevant for comparison to experiment, from computationally affordable system sizes. A simple and seemingly straightforward approach is to extrapolate from a series of finite supercell sizes to the infinite-size limit, assuming a smooth, polynomial dependence of the energy on inverse supercell size. By means of explicit density-functional theory supercell calculations and simplified electrostatic models we demonstrate that the dependence of the formation energy on supercell size can be more complex than is commonly assumed. We show that this complexity cannot be captured by the simple extrapolation approaches. In contrast, suitable correction schemes are shown to provide rapidly converging results even for 2D materials.

[1] C. Freysoldt, J. Neugebauer, A. M. Z. Tan, R. G. Hennig, Phys. Rev. B **105**, 014103 (2022).

O 30.8 Tue 12:15 GER 37

Excited state geometry relaxation of point defects in hexagonal boron nitride — •Alexander Kirchhoff, Thorsten Deilmann, and Michael Rohlfing — Westfälische Wilhelms-Universität Münster, Institut für Festkörpertheorie, Wilhelm-Klemm-Straße 10, 48149 Münster

The optical gap of pristine hexagonal boron nitride is above 5 eV and therefore in the deep UV range. Emitters in the optical regime can act as single photon sources and gained attraction due to their possible room temperature stability. However, their atomic composition is still elusive. Experiments combining spectroscopic methods to probe ground as well as excited state of defects in hBN have revealed the relevance of the dependence of optoelectronic properties on the nuclear geometry.

In our work, this dependence is studied within the framework of density functional theory and the *GW*/BSE approximation. We focus on carbon based defects in hBN and present a detailed analysis of their excitonic spectrum [1]. C_BO_N for example has a defect bound exciton at 1.5 eV. We obtain a Stokes shift of about 1 eV by calculating the energy surfaces of ground and excited state.

[1] Kirchhoff, Deilmann, Krüger and Rohlfing, Phys. Rev. B 106, 045118 (2022)

O 30.9 Tue 12:30 GER 37

Semiclassical theory of plasmons in inhomogeneous two-dimensional systems — •Tjacco Koskamp, Koen Reijnders, and Mikhail Katsnelson — Radboud University, Nijmegen, The Netherlands

We consider plasmons, collective oscillations of conduction electrons, in inhomogeneous two-dimensional systems with parabolic dispersion. In recent years, the quantum regime for plasmons has become experimentally accessible. Although these systems can be studied numerically, this approach is limited to relatively small systems. Recently, a comprehensive analytical theory for plasmons based on the semiclassical (WKB) approximation was proposed [1]. It describes plasmons in inhomogeneous three-dimensional systems, and is applicable when the inhomogeneity, in e.g. the electron density, varies smoothly.

In this talk, we extend this theory to plasmons in inhomogeneous two-dimensional systems. We consider the equation of motion for the density matrix and take the electron-electron interaction into account through the RPA. We solve this system of equations self-consistently, carefully separating the in-plane and out-of-plane degrees of freedom. In this way, the effective classical Hamiltonian for plasmons is obtained. Subsequently, we apply this theory to a scattering experiment. We first construct the classical trajectories and then use the semiclassical phase shift to compute the differential scattering cross section.

[1] K.J.A. Reijnders, T. Tudorovskiy, M.I. Katsnelson, Ann. Phys. 446, 169116 (2022)

O 30.10 Tue 12:45 GER 37

Hot electron driven charge carrier dynamics at the MoS_2/gold interface: a sum frequency generation study — •Tao Yang, Erik Pollmann, Stephan Sleziona, Peter Kratzer, Marika Schleberger, Richard Kramer Campen, and Yujin Tong — Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany

Monolayer transition metal dichalcogenides (TMDCs) have potential applications as optoelectronics and (photo)electrocatalysts due to their fascinating electronic and optical properties. Applying these extraordinary properties to build devices and catalysts, it is often necessary to bring TMDCs into contact with a metallic surface. However, the charge transfer process across the semiconductor-metal interface is still not clear. While the quench of photoluminescence spectra has been reported for monolayer TMDCs on gold, which was understood to be a charge transfer of excited electrons from TMDC monolayer into the metal, it's interesting to ask what happens when the charge carrier is excited from the metal side. Here we use an azimuthal-dependent sum frequency generation combined with a pump-probe scheme to study the effect of the selectively excited hot electrons by 800 nm pump laser on the behavior of excitons of monolayer MoS_2. Our results show that the hot electrons from the gold substrate can significantly suppress the formation of excitons.

O 30.11 Tue 13:00 GER 37

Structure and electronic-optical properties of polymeric carbon nitride — •Changbin Im, Björn Kirchhoff, and Timo Jacob — Ulm University, Institute of Electrochemistry, Ulm, Germany

Understanding of the electronic structure and optical properties of polymeric carbon nitrides (PCNs) is of key interest in order to exploit their photo-physical and photo-electrocatalytic capabilities. The numerous defects of typical PCNs, however, present a limitation to computational studies that aim to improve our fundamental understanding of this material class. Here, we demonstrate a systematic thermodynamic study and structural characterization of various heptazine based-PCN models from the viewpoint of electronic and optical properties obtained with hybrid density functional theory (DFT). Our calculations reveal the key structural factors (degree of condensation, interlayer distance, corrugation) that govern the formation of various PCN motifs and their optical properties.[1] We discuss how each of the key factors influences the electronic structure of PCNs. We also suggest the concept of exciton binding energy in PCNs and discuss the polaronic interactions between heptazine units due to the localized exciton nature. Furthermore, we disclose a failure of GGA in the description of correlated electrons that underestimates the energy of the conjugated electrons comparing hybrid DFT. From the results, we could not only deduce a more complete model for the diverse PCN motifs but could additionally derive fundamental trends for future material optimization.

[1] Im, C. et al. (2022). http://arxiv.org/abs/2208.02582 submitted.

O 31: Focus Session: Ion Beam Interaction with Surfaces and 2D Materials III

Time: Tuesday 10:30–12:45 Location: GER 38

Topical Talk O 31.1 Tue 10:30 GER 38

Ultra-low energy ion implantation of two-dimensional materials — •Hans Hofsäss[1], Felix Junge[1], Manuel Auge[1], Beata Kardynal[2], Ursel Bangert[3], Martin Wenderoth[4], and Lino Pereira[5] — [1]2nd Institute of Physics, University of Göttingen, Germany — [2]Peter Grünberg Institute, Forschungszentrum Jülich, Germany — [3]Department of Physics, University of Limerick, Ireland — [4]4th Institute of Physics, University of Göttingen, Germany — [5]Department of Physics, KU Leuven, 3001 Leuven, Belgium

Doping of two-dimensional (2D) materials by ion implantation requires unique requirements regarding ion energy, ion beam optics and sample preparation. Efficient substitutional incorporation of low energy ions into the 2D lattice requires energies around 20 eV. We use a low energy mass selected ion beam system with UHV implantation chamber. A 30 keV mass selected ion beam is guided through differential pumping stages and homogenized using a beam sweep. An area of about 1-2 cm^2 can be uniformly irradiated with these ultra-low-energy (ULE) ions with a beam current up to several microAmp. Results for doping of monolayer graphene with B^+, N^+ an P^+ ions and doping of 2D MoS$_2$ with Se$^+$ and Cr$^+$ ions will be presented. We discuss challenges for ULE ion implantation, such as non-flat substrates, ion sources and lateral selective doping. Results for analyses of the implantation efficiency and lateral doping are presented. The simulation of ULE ion implantation using novel Monte Carlo Binary Collision Approximation programs is also discussed.

O 31.2 Tue 11:00 GER 38

Low-Energy Ion Implantation with an electron beam evaporator — •Tom Weinert, Denise Jennifer Erb, Stefan Facsko, René Heller, and Ulrich Kentsch — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Deutschland

For ion implantation of thin films and in particular of two-dimensional materials, it is necessary to reduce the ion energy down to 10eV. For this purpose, we develop a a simple and robust setup via a new approach. We use an electron beam evaporator to generate the desired ions. This has the advantage of a relatively small energy distribution of the ions, and in addition numerous different metal ions can be generated. An electrostatic analyzer is used to filter out the neutral atoms and to improve the energy distribution of the ion beam to below 5eV. The used ion energy is below 1keV and is suitable for the implantation of very thin surface layers or, after further energy reduction, for implantation in two-dimensional materials. Ion implantation can change the properties of two-dimensional materials, enabling, for example, new electrical, magnetic or catalytic applications.

O 31.3 Tue 11:15 GER 38

Fabrication of 2D magnets by ion implantation of phyllosilicates — Muhammad Zubair Khan[1], Nico Klingner[2], Gregor Hlawacek[2], Aleksandar Matković[1], and •Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben, 8700 Leoben, Austria — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany

Since the first reports on intrinsically magnetic two-dimensional (2D) materials in 2017 [1,2], the price-to-pay for accessing their monolayers is still the lack of ambient stability. Recently, we demonstrated weak ferromagnetism in 2D Fe:talc at room temperature and proposed iron-rich phyllosilicates as a promising platform for air-stable magnetic monolayers [3]. Since these minerals are rather rare and since phyllosilicates are hard to synthesize, we suggest here as an alternative ion implantation to tailor the magnetic properties of the phyllosilicates. Nonmagnetic, single-crystalline bulk talc crystals [4] were implanted with 50 keV iron and cobalt ion beams at different substrate temperatures. In all cases, ultra-thin layers could be exfoliated indicating that the layered crystal structure is maintained after ion irradiation. For both ion species, the Mg-OH Raman peak showed a triplet formation implying a successful substitution of Mg by Fe or Co in the talc layers. [1] Gong, C., et al., Nature 546, 265 (2017). [2] Huang, B., et al., Nature 546, 270 (2017). [3] A. Matković, et al., npj 2D Mat. Appl. 5, 94 (2021). [4] B. Vasić, et al., Nanotechnology 32, 265701 (2021).

O 31.4 Tue 11:30 GER 38

Charge exchange of highly charged ions scattered under grazing incidence — •Matthias Werl, Anna Niggas, Friedrich Aumayr, and Richard A. Wilhelm — TU Wien, Institute of Applied Physics, Vienna, Austria

When a highly charged ion approaches a surface, electrons are resonantly captured from the material, starting at distances of $\approx 10-25$ Å above the surface. The electrons are captured into shells with $n \approx q_{in}$ (q_{in}: incident charge state), forming a hollow atom (*HA*) - a state where (mostly) high-n shells are populated. In the free case, these excited *HA*s would then decay via a combination of auto-ionization and radiative pathways, recharging the projectile in the process. At very close distances from a surface ($d_I \leq 3$ Å), another process, known as Interatomic Coulombic Decay (*ICD*), can take place. Here, the *HA* quickly decays to its ground state due to electron-electron scattering with electrons from the material.

To study the *HA*s and their free decay, neutralization via *ICD* is to be prevented. This can be achieved if the distance of closest approach is larger than d_I, which happens at very grazing angles. Previous experiments showed that only a minor fraction of charged particles survive up to the detector under an incident angle of $\alpha_{inc} = 1.6°$. Decreasing the incident angle even further ($0.1° \leq \alpha_{inc} \leq 1.0°$), more charged particles are expected to arrive at the detector.

Here, we present our setup to achieve these small incident angles with an accuracy of $\approx \pm 0.2°$ as well as first experimental results for the charge state distribution of the scattered projectiles.

O 31.5 Tue 11:45 GER 38

Green functions simulation of the energy and charge transfer between highly charged ions and 2D materials — •Michael Bonitz[1], Karsten Balzer[2], Hannes Ohldag[1], Jan-Philip Joost[1], Anna Niggas[3], and Richard Arthur Wilhelm[3] — [1]CAU Kiel, Institute for Theoretical Physics and Astrophysics — [2]CAU Kiel, Computing Center — [3]TU Wien, Institute of Applied Physics, Vienna, Austria

We have developed Nonequilibrium Greenfunctions (NEGF) - Ehrenfest dynamics simulations for the energy loss of ions that impact correlated 2D materials. An interesting prediction was an ion-induced increase of the doublon number [1]. Recently, these simulations were extended to highly charged ions and to the associated charge transfer and electron emission. We find reasonable agreement with the experimental predictions [2]. Here we discuss how these simulations can be extended to longer times and improved selfenergies via our G1-G2 scheme [3], combined with an embedding selfenergy approach [4].

[1] K. Balzer et al., Phys. Rev. Lett. 121, 267602 (2018); [2] A. Niggas et al., Phys. Rev. Lett. 129, 086802 (2022); [3] N. Schluenzen et al., Phys. Rev. Lett. 124, 076601 (2020); [4] N. Schluenzen et al., submitted for publication, arXiv:2211.09615

O 31.6 Tue 12:00 GER 38

Particle emission from 2d materials induced by highly charged ion impact — •Lucia Skopinski[1], Lars Breuer[1], Silvan Kretschmer[2], Arkady V. Krasheninnikov[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Duisburg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Two-dimensional (2d) materials such as graphene or transition metal dichalcogenides are expected to be key materials for novel applications. Defect engineering by highly charged ion (HCI) beams could be a way to modify their unique properties even further. An ion carries energy in the form of kinetic energy E_{kin} and potential energy E_{pot}, the latter corresponding to the energy required to create its respective charge state. Once the ion impinges on the surface, its energy is deposited into the solid and can lead to modifications and sputtering. However, the fundamental mechanisms of defect formation due to HCI-surface interaction are still under investigation.

Here, we discuss the emission of secondary ions and atoms as well as their velocity distribution from a substrate supported 2d material under HCI irradiation. The measured distributions allow a distinction between sputtering driven by the potential and the kinetic energy of the primary ion. The potential sputtering yield of MoS$_2$ has a similar dependence on the potential energy as the pore formation found in freestanding MoS$_2$ after irradiation with HCIs. The low velocities of the emitted particles indicate an interaction mechanism connected to electron-phonon coupling.

O 31.7 Tue 12:15 GER 38

Highly charged ion-induced electron emission from atomically thin materials — •Anna Niggas[1], Karsten Balzer[2], Matthias Werl[1], Friedrich Aumayr[1], Michael Bonitz[3], and Richard Arthur Wilhelm[1] — [1]TU Wien, Institute of Applied Physics, Vienna, Austria — [2]Computing Center of Kiel University, Kiel, Germany — [3]Kiel University, Institute for Theoretical Physics and Astrophysics, Kiel, Germany

When a highly charged ion impacts on a material surface, its potential energy, i.e., the sum of the binding energies of all missing electrons, is deposited within the very first surface layers. This, in turn, triggers many processes such as the emission of electrons. While both the electron yield and energy distribution of bulk samples have been extensively studied in the past, data for 2D materials is rather scarce. This is due to the challenging task of separating signals of the 2D material itself from its support structure. Therefore, we developed a coincidence setup correlating ions after transmission with electrons emitted from the material. This allows us to discriminate signals from the support via the ion energy loss in the sample and, consequently, to access the emission from the 2D material alone.

In this contribution we will present our recent studies on the electron emission induced by highly charged ion impact on monolayers of graphene and MoS$_2$ and their 3D counterparts. We find a 6-fold higher emission yield for graphene compared to MoS$_2$ and a vanishing contribution of $< 10\,\mathrm{eV}$ electrons for MoS$_2$. These findings are supported by simulations of the ion-induced surface charge dynamics.

O 31.8 Tue 12:30 GER 38

Light ion transmission through atomically thin material: insights from non-adiabatic first-principles simulations — •Silvan Kretschmer[1], Arkady V. Krasheninnikov[1], Anna Niggas[2], Lukas Fischer[2], and Richard A. Wilhelm[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]TU Wien, Institute of Applied Physics, Vienna, Austria

Two-dimensional materials, as surface-only targets, are ideally suited to study the neutralization and deexcitation of charged particles. Using atomistic Ehrenfest dynamics simulations we rationalize the experimental findings obtained for transmission of H$^+$ and He$^+$ through graphene and 2D-MoS$_2$. Here semi-metal and semi-conductor are chosen exemplary to explore potentially different neutralization behaviour. Changes in the electronic structure are calculated along with the energy loss and the charge transfer from the target to the projectile during the transmission and compared to the experiment. Furthermore, low-charge state ions represent a suitable model system to validate the framework of Ehrenfest dynamics to be extended to their highly charged counter parts.

O 32: Semiconductor Substrates

Time: Tuesday 10:30–12:45 Location: GER 39

O 32.1 Tue 10:30 GER 39

Progress in local growth of III/V-semiconductor structures — •Christian Bruckmann, Jürgen Bläsing, Armin Dadgar, and André Strittmatter — Otto-von-Guericke-Universität Magdeburg, PF4120 Magdeburg, Germany

We recently developed a laser-assisted metalorganic vapor phase epitaxy (LA-MOVPE) for local growth of III/V-semiconductors[1]. The principle is based on local heating of a selected growth area by high-power laser radiation. Metalorganic precursors are fed into the reactor to the locally heated area so that the chemical reactions leading to island growth are confined within the heated area. Thereby, selective area growth can be done without full wafer heating which is advantageous for heteroepitaxy of crystalline materials and monolithic III/V device integration on Si. We report on optimum conditions for homoepitaxial GaAs growth, n- and p-type doping as well as AlGaAs/GaAs heterostructures. We discuss the proper choice of precursors and lateral homogeneity of ternary layers.

[1] M. Trippel et al., "Laser-assisted local metal-organic vapor phase epitaxy", Rev. Sci. Instrum. **93**, 113904 (2022)

O 32.2 Tue 10:45 GER 39

Post-synthesis of copper nitride monolayers from copper oxide films — •Mohammadreza Rostami[1], Biao Yang[1], Francesco Allegretti[1], Lifeng Chi[2], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, Garching, 85748, Germany — [2]Institute of Functional Nano & Soft Materials, Collaborative Innovation Center of Suzhou Nano Science and Technology, Soochow University, Suzhou 215123, P. R. China

Copper nitride (CuN) thin films represent insulating layers bearing promise for decoupling functional structures from a metallic copper substrate. [1] Although the nitrogen ion bombardment method was successfully applied for the in-situ preparation of CuN monolayers on Cu surfaces, the reduced domain size limits their application potential. [2] In this work, we have grown extended monolayer CuN films on Cu (111) surfaces by ammonia-mediated post-annealing of copper oxide (CuO) thin films. Structures and properties of CuN and CuO monolayers were characterized by scanning tunneling microscopy and low-energy electron diffraction. The element exchange of nitrogen with oxygen in the respective CuN and CuO layers on Cu (111) surfaces was evidenced by X-ray photoelectron spectroscopy. This oxidation-reduction two-step strategy provides a new approach to fabricate CuN buffer layers. [1] Z. Zhao et al, Adv. Electron. Mater. 2018, 4, 1700367 [2] H. Baek et al, Appl. Phys. Lett. 91, 253106 (2007)

O 32.3 Tue 11:00 GER 39

The role of mechanical strain in rare-earth silicide monolayers on Si(111) — •Kris Holtgrewe and Simone Sanna — Justus-Liebig-Universität, Gießen, Deutschland

Rare-earth silicide (RESi$_2$) nanostructures on silicon surfaces provide a very heterogeneous class of lower-dimensional metallic systems supported by a semiconducting substrate. The RESi$_2$ monolayer is a two-dimensional semimetal, which grows on Si(111) by self-organisation. While it has intensively been studied by experimental and theoretical works, there are major misunderstandings about the mechanisms which determine the morphological details of the monolayer. In particular, many previous studies state that mechanical strain is responsible for the structural differences between the RESi$_2$ monolayer on Si(111) (buckled Si honeycomb, vacancy-free), the RESi$_{2-x}$ bulk phase (flat Si honeycomb, vacancy-rich) and the AlB$_2$ structure (flat Si honeycomb, vacancy-free). This DFT work sheds light on the stability of the established structure model of the monolayer by a combined analysis of the structural details and the electronic band structure. It proves that the buckling of the covering Si honeycomb and the lack of Si vacancies are not due to mechanical strain, but due to charge balance. In this context, the monolayer is structurally more similar to the unstrained CaSi$_2$ structure than to the strained AlB$_2$ structure, which explains its stability. It is very likely that the misinterpreted role of mechanical strain is transferable to all RESi$_2$ nanostructures.

O 32.4 Tue 11:15 GER 39

Electronic and magnetic properties of ultrathin FeBr$_2$ films grown on Bi/Si(111) — •Shigemi Terakawa[1], Jiabao Yang[1], Shinichiro Hatta[2], Hiroshi Okuyama[2], Tetsuya Aruga[2], Niels Schröter[1], and Stuart Parkin[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Graduate School of Science, Kyoto University, Kyoto, Japan

Mono and a few layers of van der Waals (vdW) magnets are promising two-dimensional (2D) materials to fabricate heterostructures with topological materials to realize novel topological phases via proximity effects, such as the quantum anomalous Hall effect. FeBr$_2$ is a layered Ising antiferromagnet, where the magnetic moments are coupled ferromagnetically in a layer and antiferromagnetically between adjacent layers. We succeeded in the epitaxial growth of ultrathin FeBr$_2$ films using molecular-beam epitaxy on Bi/Si(111) substrate. We observed insulating band structures using angle-resolved photoelectron spectroscopy (ARPES). The valence band top is located at a flat band with a binding energy of 2 eV, which is ascribed to Fe 3d orbitals. At monolayer coverage, the Fe 3d flat band does not change but dispersive bands of Br 4p at 7-8 eV are largely altered due to the disappearance of inter-layer Br-Br coupling in the monolayer film. The monolayer film shows a strong moire pattern in low-energy electron diffraction (LEED), suggesting a strong coupling between the $FeBr_2$ and Bi films. We plan to discuss the magnetic properties of the $FeBr_2$ films from the results of XMCD experiments.

O 32.5 Tue 11:30 GER 39

In situ XPS Study on ultrathin Fe_xO_y Films on $SrTiO_3$ — •Pia Maria Düring, Timo Krieg, and Martina Müller — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Oxide interfaces are emerging as one of the most interesting systems in condensed matter physics as they exhibit a multitude of physical phenomena such as 2D electron/hole gas, superconductivity, or the Spin Hall effect. One of the main processes that controls the physical properties is the oxygen exchange between the film and the substrate. The tunability of the oxygen transfer using different growth parameters opens up the possibility to unravel unexplored properties.

Using our UHV-MBE system, we grow high-quality ultrathin Fe-oxide films on $SrTiO_3$ substrates by systematically varying certain growth parameters. Performing in situ X-ray Photoelectron Spectroscopy and Low Energy Electron Diffraction enables the analysis of the electronic properties and crystalline structure of ultrathin Fe_xO_y films directly after the growth without any atmospheric contamination.

The present work discusses the effect of different growth temperatures, substrate annealing procedures, and film thicknesses of the Fe_xO_y films on the interfacial properties like oxygen vacancies. The results open up the possibility for the emergence of 2D electronic states at the interface by tuning such growth parameters.

O 32.6 Tue 11:45 GER 39

MOVPE of Stacked Quantum Dots Layers at 1250 nm Wavelength — •Ege Özmen, Armin Dadgar, and André Strittmatter — Otto von Guericke University, Magdeburg, Germany

LIDAR, light detection and ranging, is the technology to produce a 3D model of surroundings using semiconductor laser technology. In LIDAR, the return of laser pulses reflected from an object's surface is recorded in time. For optimum control of laser direction, a tightly bundled laser radiation is required. Since the light output from traditional semiconductor edge-emitting lasers is highly divergent, especially along the vertical axis, novel concepts for optical waveguides in laser diodes with lower output divergence have to be considered. Besides, as LIDAR operates in free space, a proper choice for laser wavelength has to be made. The current choice is around 905 nm wavelength which raises concerns about eye safety. Much better eye safety and therefore higher output powers could be realized if high-brilliance lasers operating at 1250 nm wavelength could be used. Here, we report on an optimization of MOVPE growth conditions to obtain up to 10-fold stacks of InGaAs quantum dots on a GaAs(001) substrate. We compare laser structures with 5-10 QD layers for static output characteristics.

O 32.7 Tue 12:00 GER 39

About the excitation of island growth orthogonal to the surface in the substrate Pb/Si(111)-(7x7) — •Paul Philip Schmidt, Lea Faber, and Regina Hoffmann-Vogel — Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany

With the increasing miniaturization of systems, the phenomena of surface diffusion is becoming more and more relevant. Pb shows anormaly fast mass transport on Si(111)-(7x7) [1,2]. For this system island growth and the behaviour of the wetting layer must be taken into account in order to understand the physical processes at the surface. We investigate the growth of the islands. Si was cleaned by rapid heating to 1200°C. Pb was deposited on the sample by evaporation at room temperature or liquid nitrogen temperature (120K). We create local imbalances of Pb to draw conclusions about diffusion and selectively trigger island growth at individual islands. While we measure the topography with non contact atomic force microscopy, we simultaneously determine the local work function difference with Kelvin probe force microscopy. Our experiments show an energy barrier before ring growth occurs. Once atoms have reached an existing island, ring growth around occurs quickly. In experiments where we do not force this the islands hardly show any growth perpendicular to the surface. Part of the Pb comes from the restructuring of the island, which initially shrinks in the xy-direction.

[1] M. Hupalo et. al. Phys. Rev. B, 23, 235443 (2007)
[2] K. L. Man et al. Phys. Rev. Lett., 101 226102 (2008)

O 32.8 Tue 12:15 GER 39

Solution-Synthesized Extended Graphene Nanoribbons Deposited by High-Vacuum Electrospray Deposition — •Sebastian Scherb[1], Antoine Hinaut[1], Xuelin Yao[2], Alicia Götz[2,3], Samir H. Al-Hilfi[2], Xiao-Ye Wang[2], Yunbin Hu[2], Zijie Qiu[2], Yiming Song[1], Klaus Müllen[2,3], Thilo Glatzel[1], Akimitsu Narita[2], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Max Plank Institute for Polymer Research, Mainz, Germany — [3]Department of Chemistry, Johannes Gutenberg University Mainz, Mainz, Germany

Solution-synthesized graphene nanoribbons (GNRs) can facilitate various interesting structures or functionalities, like non-planarity and thermo-labile functional groups, which can be difficult to access via on-surface synthesis [1,2]. However, their deposition and thus study on surfaces remains challenging.

Here, we show high-vacuum electrospray deposition (HVESD) of well-elongated solution-synthesized GNRs on metallic and non-metallic surfaces in UHV. Thereby, we compare three distinct GNRs, exhibiting different average lengths, functional groups, and edge structures. nc-AFM studies at room temperature combined with Raman spectroscopy allow the characterization of individual GNRs and confirm their chemical integrity [3].

[1] Narita et al. Nature Chemistry 6 (2014).
[2] Narita et al. Chemical Science 10 (2019).
[3] Scherb et al. accepted in ACS Nano.

O 32.9 Tue 12:30 GER 39

Ultra-thin Noble Metal Films on Superconductors — •Christian von Bredow, Philip Beck, Lucas Schneider, Jens Wiebe, and Roland Wiesendanger — Department of Physics - University of Hamburg, Hamburg, Germany

Magnet-superconductor hybrid systems involving Rashba-split surface states proximitized by a superconducting substrate are promising platforms for the realization of topological superconductivity [1,2,3]. To that end, a large gap of the superconductor, strong spin-orbit coupling, and a high surface quality that allows for the manipulation of individual magnetic atoms using the tip of a scanning tunneling microscope are strongly desired. In order to engineer a system with the desired properties we investigate the growth and surface-state dispersion of thin noble metal films on the (110)-surface of the elemental superconductor with the highest critical temperature, niobium. Starting from a few monolayer thickness, we observe the well known quasiparticle interference of the Shockley (111) surface state. Bias-dependent data is used to extract the layer-thickness dependence of the band bottom and the effective electron mass.

[1] A. C. Potter et al., Phys. Rev. B 85, 094516 (2012).
[2] A. Palacio-Morales et al., Science Advances 5 eaav6600 (2019)
[3] T. Tomanic et al., Phys. Rev. B 94, 220503 (2016).

O 33: Spins on Surfaces at the Atomic Scale III

Time: Tuesday 10:30–13:00 Location: REC C 213

Topical Talk O 33.1 Tue 10:30 REC C 213

Fermi liquids, Luttinger integrals, topological invariants … and magnetic molecules — •Rok Zitko[1,2], German G. Blesio[1,3], Luis O. Manuel[3], and Armando A. Aligia[4] — [1]Jozef Stefan Institute, Ljubljana, Slovenia — [2]Faculty of Mathematics and Physics, University of Ljubljana, Slovenia — [3]Instituto de Fisica Rosario (CONICET) and Universidad Nacional de Rosario, Argentina — [4]INN CNEA-CONICET, Centro Atomico Bariloche and Instituto Balseiro, Bariloche, Argentina

The ground state of a system of interacting fermions is often a Fermi liquid with elementary excitations that are in a one-to-one correspondence with those of a non-interacting Fermi gas. A key idea in Landau's theory is the adiabatic connection between the interacting and the non-interacting system. The adiabatic connection does not, however, always exist and there are several impurity problems where the ground state is known to be a Fermi liquid that is not of the Landau type. I will present the case of the two-channel S=1 Kondo model with single-ion magnetic anisotropy which has a topological quantum phase transition separating two different Fermi-liquid phases. I will discuss how the conservation laws constrain the Luttinger integrals so that their linear combinations become topological invariants, and how the modified Friedel sum rules lead to a peculiar variation of the impurity spectral function. I will then show that the tunneling spectra of iron phthalocyanine molecules on Au(111) surface and of nickelocene molecules on Cu(100) surface can be consistently interpreted in the framework of non-Landau Fermi liquid theory.

O 33.2 Tue 11:00 REC C 213

Locally driven quantum phase transition cascades in a strongly correlated molecular monolayer — Soroush Arabi[1,2,3], Taner Esat[2,5], Aizhan Sabitova[2,5], Yuqi Wang[2,3], Hovan Lee[6], Cedric Weber[6], Kern Klaus[3,4], F. Stefan Tautz[1,2,5], Ruslan Temirov[2,7], and •Markus Ternes[1,2,5] — [1]Institute of Physics IIB, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter-Grünberg-Institute (PGI 3), Research Center Jülich, 52425 Jülich, Germany — [3]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [4]Institut de Physique, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [5]Jülich Aachen Research Alliance, 52425 Jülich, Germany — [6]King's College London, Theory and Simulation of Condensed Matter, London WC2R 2LS, UK — [7]Institute of Physics II, University of Cologne, 50937 Cologne, Germany

The molecular monolayer of 1,4,5,6-naphthalene tetracarboxylic acid dianhydride on Ag(111) creates a perfectly ordered lattice of π-conjugated organic molecules. Using a movable atomically sharp electrostatic gate we drive this lattice of strongly correlated electrons through a cascade of quantum phase transitions. Performing spectroscopic imaging with sub-Angstrom resolution, we show that as the gate field is increased, the molecular building blocks change from a Kondo-screened to a paramagnetic phase one by one, enabling us to reconstruct their complex interactions in detail. We anticipate that the supramolecular nature of the system will, in future, allow engineering quantum correlations in arbitrary patterned structures.

O 33.3 Tue 11:15 REC C 213

Engineering antiferromagnetic spin coupling in carbon based nanostructures — •Elia Turco[1], Nils Krane[1], Fupeng Wu[2], Michal Juricek[3], Xinliang Feng[2], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa Swiss Federal Laboratories for Materials Science and Technology, Duebendorf, Switzerland — [2]Faculty of Chemistry and Food Chemistry, and Center for Advancing Electronics Dresden, Technical University of Dresden, Germany — [3]Department of Chemistry, University of Zurich, Switzerland

On-surface synthesis offers the possibility to engineer atomically precise nanogaphenes (NGs) with intrinsic magnetic ground states. Unlike atomic magnets, unpaired π-electrons are highly delocalized and prone to hybridize forming entangled quantum states, which are the main requisite for the emerging quantum technologies. Zigzag-edged triangular NGs are regarded as prototypical magnetic building blocks, hosting a total spin S that scales with molecular size [1]. In this contribution, we will present the on-surface synthesis and scanning probe microscopy & spectroscopy of the two smallest $S = 1/2$ and $S = 1$ triangulenes on a Au(111) surface, where the Kondo screening of the unpaired spins is a direct evidence of their magnetic ground state. Connecting the two $S = 1/2$ and $S = 1$ building blocks into homo- and hetero-dimers an -trimers, we realize multilevel quantum systems with increasing complexity, characterized by multiple inelastic spin excitations. The significant hybridization of the unpaired π-electrons results in strong quantum correlations, which have never been achieved for equivalent atomic systems. [1] J.Su et al. Angew. Chem. 132 (2020)

O 33.4 Tue 11:30 REC C 213

Moiré tuning of spin excitations: individual Fe atoms on MoS_2/Au(111) — •Christian Lotze[1], Sergey Trishin[1], Nils Bogdanoff[1], Felix von Oppen[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Germany — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, Germany

Magnetic adatoms on properly designed surfaces constitute exquisite systems for addressing, controlling, and manipulating single quantum spins. Here, we show that monolayers of MoS_2 on a Au(111) surface provide a versatile platform for controllably tuning the coupling between adatom spins and substrate electrons. Even for equivalent adsorption sites with respect to the atomic MoS_2 lattice, we observe that Fe adatoms exhibit behaviors ranging from pure spin excitations, characteristic of negligible exchange and dominant single-ion anisotropy, to a fully developed Kondo resonance, indicating strong exchange and negligible single-ion anisotropy. This tunability emerges from a moiré structure of MoS_2 on Au(111) in conjunction with pronounced many-body renormalizations. We also find striking spectral variations in the immediate vicinity of the Fe atoms, which we explain by quantum interference reflecting the formation of Fe-S hybrid states despite the nominally inert nature of the substrate. Our work establishes monolayer MoS_2 as a tuning layer for adjusting the quantum spin properties over an extraordinarily broad parameter range. The considerable variability can be exploited for quantum spin manipulations.

O 33.5 Tue 11:45 REC C 213

Absence of the Kondo effect for Co on Cu(111) — Neda Noei[1], Roberto Mozara[2], Ana M. Montero[3], Sascha Brinker[3], Niklas Ide[1], Filipe S. M. Guimaraes[3], Alexander I. Lichtenstein[2], Richard Berndt[1], Samir Lounis[3], and •Alexander Weismann[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

The zero-bias anomaly in conductance spectra of single Co atoms on Cu(111) observed at ≈ 4 K, which has been interpreted as being due to a Kondo resonance, is strongly modified when the Co atoms are attached to monatomic Cu chains. Scanning tunneling spectra measured at 340 mK in magnetic fields exhibit all characteristics of spin-flip excitations. Their dependence on the magnetic field reveals a magnetic anisotropy and suggests a non-collinear spin state indicating that spin-orbit coupling (SOC), which has so far been neglected in theoretical studies of Co/Cu(111), has to be taken into account. According to our density functional theory and multi-orbital quantum Monte Carlo calculations SOC suppresses the Kondo effect for all studied geometries. The interpretation of the zero-bias anomaly in terms of a Kondo resonance is apparently incorrect.

O 33.6 Tue 12:00 REC C 213

Are excitations of the 4f magnetic moment visible to the scanning tunneling spectroscopy? — Daria Kyvala and •Jindrich Kolorenc — Institute of Physics (FZU), Czech Academy of Sciences, Praha, Czech Republic

The inelastic electron tunneling spectroscopy (IETS) has repeatedly proved useful for investigation of spin excitations in transition-metal atoms on surfaces [1,2]. Analogous observations of magnetic excitations in rare-earth atoms remained elusive, the reasoning behind it being that the 4f states that carry the magnetic moment are compact, buried in the atomic core, and the tunneling through a rare-earth atom proceeds via outer, more diffuse orbitals like 5d or 6s. Recently, the exchange coupling between the spin in these outer orbitals and the 4f magnetic moment was observed in IETS as an excitation in the 50–200 meV range [3]. In the same time, some excitations at lower energies were also seen. Employing a variant of the cotunneling theory [4,5] we demonstrate these excitations to be the elusive crystal-field excitations of the 4f magnetic moment. The selection rules prevent the IETS from detecting enough transitions to fully determine the crystal field by itself, but the visible transitions can be used in conjunction with the x-ray absorption spectra [6] to refine the existing estimates of the crystal field. — [1] A. J. Heinrich *at al.*, Science **306**, 466 (2004); [2] C. F. Hirjibehedin *at al.*, Science **317**, 1199 (2007); [3] M. Pivetta *at al.*, PRX **10**, 031054 (2020); [4] F. Delgado and J. Fernández-Rossier, PRB **84**, 045439 (2011); [5] C. Wäckerlin *et al.*, ACS Nano **16**, 16402 (2022); [6] R. Baltic *et al.*, PRB **98**, 024412 (2018).

O 33.7 Tue 12:15 REC C 213

Tuning the magnetic anisotropy of two coupled spins in a dinuclear Co(II) complex — Chao Li[1], Roberto Robles[2], Nicolas Lorente[3], Alexander Weismann[1], Richard Berndt[1], and •Manuel Gruber[4] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), 20018 Donostia-San Sebastián, Spain — [3]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastian, Spain — [4]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany

The magnetic properties of transition-metal ions are often described using a phenomenological spin Hamiltonian, which suggests that $S = 1/2$ metal ions are isotropic. We investigated a di-nuclear Co(II) complex on Au(111) with low-temperature scanning tunneling microscopy, X-ray magnetic circular dichroism, and density functional theory. The antiferromagnetically coupled Co spins preferentially align along the axis connecting the two Co(II) ions. The magnetic anisotropy is sizable and may be tuned by varying the electronic coupling of the Co(II) ions with the metal electrodes through manipulation of peripheral groups and by approaching the tip toward the complex. These findings may help better describing the magnetic properties of adsorbed molecules, in particular $S = 1/2$ ions, which are viewed as prototypical systems for quantum operations. Funding from the CRC 1242 is acknowledged.

O 33.8 Tue 12:30 REC C 213

Moiré - induced renormalization of singlet-triplet excitations in antiferromagnetically coupled Mn atoms on MoS_2/Au(111) — •Sergey Trishin[1], Christian Lotze[1], Friedemann Lohss[1], Giada Franceschi[1], Leonid I. Glazman[2], Felix von Oppen[3], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Department of Physics, Yale University, New Haven, Connecticut 06520, USA — [3]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

The properties of single magnetic atoms can change drastically upon adsorption on a surface, for example due to Kondo-like exchange coupling. The magnitude of these interactions can be tuned by a moiré patterned surface [1]. Here, we investigate single Mn atoms and dimers on single-layer molybdenum disulfide grown on a Au(111) substrate. The resulting moiré structure enables variations of the Kondo exchange coupling strength. By additionally varying the spacing between single atoms, we can investigate their properties in the direct and indirect exchange coupling regime. We find that at sufficiently close spacings, the Mn atoms form a non-magnetic singlet ground state. However, the singlet-triplet excitation energies vary strongly depending on the dimer location on the moiré structure. We ascribe these variations to a renormalization of the anti-ferromagentic exchange coupling strength. [1] S. Trishin and C. Lotze and N. Bogdanoff and F. von Oppen and K.J. Franken, Phys. Rev. Lett. **127**, 236801 (2021)

O 33.9 Tue 12:45 REC C 213

Stochastic dynamics of individual and coupled orbital memory on black phosphorus — •Hermann Osterhage, Werner M. J. van Weerdenburg, Niels P. E. van Mullekom, Ruben Christianen, Kira Junghans, Eduardo J. Domínguez Vázquez, Hilbert J. Kappen, and Alexander A. Khajetoorians — Radboud University, Nijmegen, The Netherlands

Recently, the dynamics of Co atoms adsorbed on a black phosphorus (BP) surface were shown to emulate a Boltzmann machine (BM) [1]. The BM relies on a tunable multi-well energy landscape, realized in the stochastic switching of coupled atoms which exhibit orbital memory [2]. Stochastic switching between orbital memory states can be induced using scanning tunneling microscopy (STM). The system response depends on interatomic distances and is adaptable to the position of the STM tip and to the applied DC bias [2].

Here, we present the response of individual and coupled Fe and Co atoms on BP to AC input voltages (i.e. frequency and amplitude response), measured using STM down to millikelvin temperatures. We find a frequency response of the orbital memory of single atoms. The changes in orbital state population with varying AC frequency can be derived from the switching dynamics in the DC case. The interatomic coupling is discussed based on changes in switching rates conditioned on the state of a second atom. Also the AC stochastic response in the multi-well limit will be discussed.

[1] B. Kiraly et al., Nat. Nanotechnol. 16, 414 (2021).

[2] B. Kiraly et al., Nat. Commun. 9, 3904 (2018).

O 34: Ultrafast Electron Dynamics at Surface and Interfaces III

Time: Tuesday 10:30–13:15 Location: TRE Phy

O 34.1 Tue 10:30 TRE Phy

Resolving Intervalley Exciton Couplings in Atomically Thin Semiconductors with Multidimensional Spectroscopy — •Lawson Lloyd[1,2], Ryan Wood[2], Fauzia Mujid[2], Siddhartha Sohoni[2], Karen Ji[2], Po-Chieh Ting[2], Jacob Higgins[2], Jiwoong Park[2], and Gregory Engel[2] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]The University of Chicago, Chicago, IL, USA

Atomically thin transition metal dichalcogenides (TMDs) have emerged as promising candidates for next-generation optoelectronic applications. In particular, an optically addressable “valley” degree of freedom at the K/K’ points can be used to store and readout information by exploiting the valley-dependent chiral optical selection rules. However, intervalley coupling after optical excitation leads to a loss of the valley polarization on ultrafast timescales. Identifying the microscopic mechanisms driving valley depolarization is therefore critical to advancing useful applications.

Here, leveraging multidimensional electronic spectroscopy, we track the exciton dynamics and couplings in large-area monolayer MoS_2 with femtosecond and valley resolution. We show that intervalley coupling between exciton states occurs both on the timescale of excitation (∼10 fs) and with minimal dependence on the excitation fluence, temperature, or sample grain size. These results shed light on the strong many-body interactions governing the femtosecond exciton dynamics in TMDs and the factors limiting the realization of novel technologies built around the valley degree of freedom.

O 34.2 Tue 10:45 TRE Phy

Electron dynamics after a spin- and valley-polarized electronic excitation in WS_2 — •Lasse Münster[1], Sarah Zajusch[1], Raul Perea-Causin[1], Samuel Brem[1], Katsumi Tanimura[1], Jens Güdde[1], Yaroslav Gerasimenko[2], Rupert Huber[2], Ermin Malic[1], Ulrich Höfer[1], and Robert Wallauer[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Fachbereich Physik, Universität Regensburg, Germany

The excitonic landscape of monolayer transition metal dichalcogenides (TMDCs) comprises optically accessible bright excitons as well as spin- and momentum-forbidden dark excitonic states. We image the formation process of these states after optical excitation on an ultrashort timescale with time-resolved momentum microscopy.

We excite monolayer WS_2 resonantly to the A 1s exciton with circular polarized light. This excitation leads to a population, which is located purely within the K valley for one helicity and in the K’ valley for the other helicity. In the case of an excitation at K, electron scatter to K’ and Σ by spin-conserving processes within a few tens of femtoseconds. Furthermore, we observe the formation of spin-forbidden excitons in the K valley and electron scattering towards Σ’.

Both of these processes involve a spin-flip and are significantly slower (50 - 100 fs).

O 34.3 Tue 11:00 TRE Phy

Influence of the substrate dielectric permittivity on ultrafast quasiparticles dynamics in WS_2 monolayers — •Subhadra Mohapatra^{1,2}, Lukas Gierster^{1,2}, Stefano Calati^{1,2}, Nicholas Michael Olsen^{3}, Quiyang Li^{3}, Xiaoyang Zhu^{3}, and Julia Stähler^{1,2} — ^{1}Humboldt-Universität zu Berlin, Institut für Chemie — ^{2}Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abt. Physikalische Chemie, Berlin, Germany — ^{3}Columbia University

In our recent fluence-and photon energy-dependent studies [1,2] of quasiparticle dynamics in WS_2 monolayers on fused silica (FS) and Si-SiO_2 substrates, we observed that excitonic screening reduces the binding energy of the excitons, however the role of screening due to substrates and the quantitative nature of dynamic screening due to excitons remained inconclusive. On further investigation of such fluence-dependent quasiparticle dynamics studies using a higher dielectric permittivity of a sapphire substrate, we found that scattering rates, relaxation time constants, and band gap renormalization are not influenced by the dielectric permittivity. On the contrary, the dynamic screening parameter of the excitons is approximately two times higher in FS than Sapphire and Bohr radius is approximately 2.5 % higher in sapphire than for FS, which must be a direct consequence of the increased dielectric permittivity likely leading to more delocalized excitons.

References:

[1] Calati et al. PCCP 23(39) (2021).

[2] Calati et al. arXiv:2204.02125 (2022).

O 34.4 Tue 11:15 TRE Phy

Probing the ultrafast hole-transfer mechanism in a twisted TMD heterostructure — •Marcel Reutzel^{1}, Jan Philipp Bange^{1}, David Schmitt^{1}, Wiebke Bennecke^{1}, Giuseppe Meneghini^{2}, AbdulAziz AlMutairi^{3}, Daniel Steil^{1}, Sabine Steil^{1}, R. Thomas Weitz^{1}, Samuel Brem^{2}, G. S. Mathijs Jansen^{1}, Stephan Hofmann^{3}, Ermin Malic^{2}, and Stefan Mathias^{1} — ^{1}I. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany — ^{2}Fachbereich Physik, Philipps-Universität, 35032 Marburg, Germany — ^{3}Department of Engineering, University of Cambridge, Cambridge CB3 0FA, U.K.

In type-II band aligned TMD heterostructures, long-lived interlayer excitons (ILX) can be formed via two different processes: Optically excited intralayer excitons either transfer the exciton's electron or hole component across the interface. Using momentum microscopy [Rev. Sci. Ins. 91, 063905 (2020)], we have shown that the transfer of the exciton's electron proceeds via exciton-phonon scattering and layer hybridized Σ-excitons [Schmitt *et al.*, Nature 608, 499 (2022)].

In this contribution, we show that the Coulomb correlation between the exciton's hole and electron can be used to probe the hole-transfer dynamics: The intralayer exciton's hole transfers from the VBM of MoS_2 into the VBM of WSe_2, which is imprinted onto the photoemission signal as an apparant upshift of the mean photoelectron energy. Our analysis provides new insights on the ultrafast hole-transfer mechanism in the WSe_2/MoS_2 heterostructure, and, more generally, on the photoemission signature of Coulomb correlated electron-hole pairs.

O 34.5 Tue 11:30 TRE Phy

Resolving momentum-dependent phonon buildup at a 1T-TiSe2 surface using diffuse scattering in ultrafast LEED — •Felix Kurtz^{1}, Tim Dauwe^{1}, Sergey Yalunin^{1}, Gero Storeck^{2}, Jan Gerrit Horstmann^{1}, Hannes Böckmann-Clemens^{1}, and Claus Ropers^{1,2} — ^{1}Max Planck Institute for Multidisciplinary Sciences, Am Fassberg 11, D-37077 Göttingen — ^{2}4th Physical Institute, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Electron-phonon and phonon-phonon couplings govern the energy flow into and within the lattice following femtosecond laser excitation. The resulting transient phonon population can be directly deduced from momentum-resolved maps in ultrafast electron diffuse scattering [1]. Here, we employ ultrafast low-energy electron diffraction (ULEED) [2] to investigate structural dynamics and pathways for energy relaxation in the optically-excited charge-density-wave phase of 1T-$TiSe_2$. By analyzing the diffuse scattering background, we track the nonequilibrium evolution of the phonon population and observe strongly momentum-dependent rise times. Specifically, we find a rapid buildup of zone-boundary phonons within few picoseconds, followed by a substantially slower generation of low-energy zone-center acoustic phonons. Our findings are corroborated by *ab-initio* DFT calculations of phonon-phonon scattering rates. We believe that the presented approach is generally applicable to a variety of systems and provides fundamental insights into surface phonon dynamics and relaxation pathways.

[1] L. P. René de Cotret, *et al.*, Phys. Rev. B 100, 214115 (2019)

[2] G. Storeck, *et al.*, Structural Dynamics 7, 034304 (2020)

Topical Talk O 34.6 Tue 11:45 TRE Phy

Photoemission orbital tomography for excitons — •Peter Puschnig, Andreas Windischbacher, Melvin Hodžić, and Christian S. Kern — Institute of Physics, NAWI Graz, University of Graz, Austria

In photoemission orbital tomography (POT), the photoemission angular distribution (PAD) of oriented molecular layers is interpreted in terms of the Fourier transform of the initial molecular orbital from which the electron is emitted. Recently, it has been demonstrated that POT can in principle also be applied to optically excited states using a femtosecond pump-probe setup, which images the excited electron-hole pairs of a system, the excitons, on ultrafast time scales [1]. However, a rigorous and generally applicable connection between the measured PAD and the spatial structure of the excitons is lacking. By considering the expansion of the exciton wave function in the product basis of valence and conduction state orbitals, as typically done when solving the electron-hole Bethe-Salpeter equation or Casida's equations in the framework of TDDFT, we demonstrate in this contribution that the PAD is given by the Fourier transform of a coherent sum of the electronic part of the exciton wave function. This relation, which is based on a plane wave final state, as well as the unexpected consequences of the hole for the measured kinetic energy spectrum an exciton is illustrated for a series of organic molecules in the gas phase for which the PAD is also simulated explicitly, and without resorting to a plane-wave final state, by means of a real-time, real-space TDDFT approach.

[1] Wallauer et al., Science 371, 1056-1059 (2021).

O 34.7 Tue 12:15 TRE Phy

Ultrafast lattice dynamics of Niobium diselenide ($2H$-$NbSe_2$) — •Victoria C. A. Taylor^{1}, Yoav William Windsor^{1,2}, Hyein Jung^{1}, and Ralph Ernstorfer^{1,2} — ^{1}Fritz Haber Institute — ^{2}TU Berlin

Within the transition metal dichalcogenide family, $2H$-$NbSe_2$ is unusual as it exhibits metallic, charge density wave (CDW), and superconducting phases, evidencing strong electron-lattice interactions. Ultrafast techniques enable investigation of such interactions on femtosecond timescales, and several studies have investigated the ultrafast electronic response of $2H$-$NbSe_2$. However, none have directly probed the ultrafast response of the lattice. We present a femtosecond electron diffraction (FED) study on $2H$-$NbSe_2$ in its metallic phase, probing both coherent and incoherent phononic responses that result from electron-phonon and phonon-phonon scattering. From these data we explore these processes and the associated timescales.

O 34.8 Tue 12:30 TRE Phy

Non-equilibrium dynamics of bulk VSe2 — •Wibke Bronsch^{1}, Manuel Tuniz^{2}, Denny Puntel^{2}, Alessandro Giammarino^{2}, Fulvio Parmigiani^{1,2}, and Federico Cilento^{1} — ^{1}Elettra-Sincrotrone Trieste, Trieste, Italy — ^{2}Università degli Studi di Trieste, Trieste, Italy

By means of time- and angle-resolved photoemission spectroscopy (tr-ARPES), we investigate the effect of optical excitation on the electronic properties of the transition metal dichalcogenide VSe2. The electronic band structure of VSe2 has recently been subject of investigation ranging from the bulk to the monolayer regime, in search for the manifestation of the opening of a band gap in its CDW phase [1,2]. However, at present, only a few studies on the effect of an ultrafast optical excitation are available [1,3]. In our contribution we present a study on the bulk material. By selecting the polarization of the probe pulses, tr-ARPES allows us to disentangle states with different orbital character, originating from the V and Se valence bands. Our tr-ARPES data show indication for a novel photoinduced state near the Fermi level, lasting for several picoseconds after photoexcitation.

[1] Biswas et al., Nano Letters 21, 1968-1975 (2021).

[2] Umemoto et al., Nano Research 12, 165-169 (2019).

[3] P. Majchrzak et al., Phys. Rev. B 103, L241108 (2021).

O 34.9 Tue 12:45 TRE Phy

Ultrafast charge separation and charge density wave suppression in monolayer $TiSe_2$ on graphite — •Sebastian Buchberger^{1,2}, Charlotte Sanders^{3}, Yu Zhang^{3}, Emma

Springate[3], Paulina Majchrzak[4], Jill Miwa[4], Philip Hofmann[4], Søren Ulstrup[4], and Phil D. C. King[1] — [1]University of St Andrews, UK — [2]MPI for Chemical Physics of Solids, Dresden, Germany — [3]Central Laser Facility, UK — [4]Aarhus University, Denmark

The properties of two-dimensional materials and their heterostructures are often governed by the interplay of several coexisting interactions which can be difficult to disentangle in equilibrium. Time and angle resolved photoelectron spectroscopy (trARPES) is emerging as a powerful method to investigate such systems, allowing the observation of ultrafast processes such as the buildup of charge screening[1], optically induced bandgap renormalisation[2] and interlayer charge separation[3]. Here we present a trARPES study on monolayer $TiSe_2$ grown epitaxially on graphite. Monolayer $TiSe_2$ is a small indirect bandgap semiconductor that exhibits an unconventional charge density wave (CDW) in its ground state, whose origin and nature are still not fully established[4]. We study how the electronic structure evolves upon photoexcitation, tracking band shifts and spectral weight variations to disentangle charge separation, screening, and dynamical suppression of the CDW.

[1]T. Rohwer et al., Nature 471, 490-493 (2011), [2]S. Ulstrup et al., ACS Nano 10, 6315-6322 (2016), [3]S. Aeschlimann, Sci. Adv. 6, eaay0761 (2020), [4]P. Chen et al., Nat. Commun. 6:8943 (2015)

O 34.10 Tue 13:00 TRE Phy

Manipulation of the charge-density-wave in VTe2 by femtosecond light pulses — •Manuel Tuniz[1], Wibke Bronsch[2], Denny Puntel[1], Giovanni Di Santo[2], Luca Petaccia[2], Davide Soranzio[3], Davide Bidoggia[1], Maria Peressi[1], Fulvio Parmigiani[1,2], and Federico Cilento[2] — [1]Dipartimento di Fisica, Università degli Studi di Trieste, Italy — [2]Elettra - Sincrotrone Trieste S.C.p.A., Italy — [3]Institute for Quantum Electronics, ETH Zurich, 8093 Zurich, Switzerland

Comparing equilibrium and out-of-equilibrium angle-resolved photoemission spectroscopy (ARPES and tr-ARPES), we investigate the effect of an optical excitation on the electronic properties of the charge-density wave (CDW) system VTe2. Recently, the modification of the material's electronic structure triggered by CDW formation has been discussed because the strongly orbital-dependent changes may give rise to a topological change in specific bands [1]. In our contribution we show clear modifications to the electronic band structure of VTe2 induced by the emergence of the CDW phase. Moreover, our tr-ARPES experiments open the possibility to perturb the CDW phase and study the relaxation dynamics of this non-equilibrium state to the ground state of the system.

[1] Mitsuishi, N. et al. Nat Commun 11, 2466 (2020)

O 35: Focus Session: Frontiers of Electronic-Structure Theory III (joint session O/HL)

Time: Tuesday 10:30–12:45 Location: TRE Ma

O 35.1 Tue 10:30 TRE Ma

Two-component GW implementation for molecular valence excitations — •Qinglong Liu, Ramón L. Panadés-Barrueta, and Dorothea Golze — Chair of Theoretical Chemistry, Technische Universit at Dresden, 01062 Dresden, Germany

We present an all-electron GW implementation for the computation of charged molecular excitations, that includes scalar relativistic effects and spin-orbit coupling (SOC). Our method is based on a two-component (2c) approach, which can process 2c spinors and their corresponding eigenvalues from different levels of theory. The relativistic input for our 2c GW calculation is obtained in two ways: One approach is a non-self-consistent second variation SOC scheme, i.e. a scalar relativistic (SR) calculation is performed followed by an expansion of the spinors on top of the SR eigenvectors [1]. Another approach is the spinors and their eigenvalues are obtained by running a self-consistent relativistic DFT calculation with the X2C method [2]. Our algorithm has been implemented in the FHI-aims program package, which is based on numeric atom-centered orbitals (NAOs). In our 2c GW algorithm we combine the all-electron NAO scheme with the resolution of the identity technique based on the Coulomb metric (RI-V) and use the analytical continuation to evaluate the G_0W_0 self energy. We present results for the numerical validation of our implementation and for the influence of the relativistic input (second variation SOC vs X2C) on the valence excitations of small heavy molecules.

[1] W. Huhn and V. Blum, Phys. Rev. Materials 1, 033803 (2017)
[2] M. Iliaš and T. Saue, J. Chem. Phys. 126, 064102 (2007)

O 35.2 Tue 10:45 TRE Ma

Screened potential in two-dimensional GW calculations within the LAPW framework — •Ben Alex, Sven Lubeck, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

To calculate two-dimensional (2D) materials in a three-dimensional periodic code, one has to consider periodically repeated layers. The calculation of quasiparticle energies for 2D materials within the GW approximation requires the introduction of a 2D cutoff for the Coulomb potential as the layers would otherwise interact with each other. This cutoff leads to a stronger q dependence of the dielectric function around $q = 0$ which requires much denser sampling of the first Brillouin zone. In order to address this issue, an analytic expression for the dielectric function was previously derived for a plane-wave basis [1]. This expression is then integrated numerically in a small region around $q = 0$. The goal of this work is to adapt this technique to the linearized augmented planewave + local-orbital (LAPW+lo) basis as implemented in the full-potential all-electron code `exciting`. We show that also in our case, we obtain a significant computational speedup. Furthermore, this approach is compared with an approach where the dielectric function is interpolated to a denser q-grid.

[1] F. A. Rasmussen et al., Phys Rev B 94, 155406 (2016).

O 35.3 Tue 11:00 TRE Ma

GW multipole approach for the frequency description of the dielectric screening — •Claudia Cardoso[1], Dario A. Leon[2], Andrea Ferretti[1], Daniele Varsano[1], and Elisa Molinari[1] — [1]S3 Centre, Istituto Nanoscienze, CNR, 41125, Modena (Italy) — [2]Department of Mechanical Engineering and Technology Management, Norwegian University of Life Sciences, 1430, Ås (Norway)

In the present work, we discuss a numerical approach for GW calculations that takes into account the frequency dependence of the screening via a multi-pole approximation (MPA), an accurate and efficient alternative to current full-frequency methods, that overcomes several limitations of the plasmon pole approximation (PPA).

MPA was recently developed and validated for semiconductors[1]. We now extend the use of MPA to metallic systems by optimizing the frequency sampling for these class of materials and propose a simple method to include the zero q limit of the intra-band contributions. The good agreement between MPA and full frequency results for the calculations of quasi-particle energies, polarizability, self-energy and spectral functions in different metallic systems confirms the accuracy and computational efficiency of the method. Finally, we discuss the physical interpretation of the MPA poles through a comparison with experimental electron energy loss spectra for Cu.

[1] D. A. Leon, C. Cardoso, T. Chiarotti, D. Varsano, E. Molinari, A. Ferretti, Phys. Rev. B 104, 115157

Topical Talk O 35.4 Tue 11:15 TRE Ma

Towards low-scaling GW calculations for 2D materials — •Jan Wilhelm — Institute of Theoretical Physics, University of Regensburg

Semiconducting two-dimensional materials are an ideal platform to study excitons thanks to the strong exciton binding energy and good experimental accessibility of the excitons. The GW+Bethe-Salpeter approach (GW+BSE) has been successful in analyzing excitons in single-layer 2D materials [1], but the application of GW+BSE is challenging for 2D double layers and moiré structures [2]. This is because the large unit cells in these structures contain hundreds to thousands of atoms, resulting in a high computational cost for GW+BSE calculations. In this talk, I will present a low-scaling GW algorithm for 2D materials that potentially allows for the inclusion of more than a thousand atoms in the simulation [3]. This algorithm is based on localized basis functions and can handle periodic boundary conditions and the divergence of Coulomb interactions in the Brillouin zone. I will present first benchmark calculations.

[1] D. Y. Qiu, F. H. da Jornada, S. G. Louie, PRL 111, 216805 (2013). [2] Nat. Phys. 17, 720 (2021), Nature 608, 499 (2022), Science

376, 406 (2022), Nature 603, 247 (2022). [3] J. Wilhelm, D. Golze, L. Talirz, J. Hutter, C. Pignedoli, JPCL 9, 306 (2018), J. Wilhelm, P. Seewald, D. Golze, JCTC 17, 1662 (2021).

15 min. break

O 35.5 Tue 12:00 TRE Ma

Accelerating core-level GW calculations by combining the contour deformation with the analytic continuation of W — •Ramón L. Panadés Barrueta and Dorothea Golze — Theoretische Chemie, Technische Universität Dresden, Bergstr. 66c, 01062 Dresden, Deutschland

Many-body methods, like the GW approximation, have recently proven to be a highly effective tool for computing core-level excitations [1]. In particular, the contour deformation (CD) is an efficient, scalable and numerically stable approach that has enabled core-level calculations on systems up to 100 atoms [2]. In this work, we reduce the scaling of CD applied to core-levels from $O(N^5)$ to $O(N^4)$, using an analytic continuation of the screened Coulomb interaction W [3]. The new method (CD-WAC) has been implemented in FHI-aims. CD-WAC has been extensively tested on well established benchmark sets like the GW100 and the CORE65, reporting MAEs of less than 5 meV with respect to CD. The theoretical scaling has been confirmed by performing scaling experiments on large acene chains and amorphous carbon. Speedups of 5 times have been attained with CD-WAC for the largest systems.
[1] D. Golze, M. Dvorak, and P. Rinke. Front. Chem., 7:377, 2019.
[2] D. Golze, J. Wilhelm, M.J. Van Setten, and P. Rinke. J. Chem. Theory Comput., 14(9):4856-4869, 2018.
[3] I. Duchemin and X. Blase. J. Chem. Theory Comput., 16(3):1742-1756, 2020.

O 35.6 Tue 12:15 TRE Ma

Many-Body Effects of Metals Investigated by Means of the GW Method — •Zimo Zhou, Nakib Protik, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Even if semilocal exchange-correlation functionals of density-functional theory (DFT) can capture the overall band structure of many metals well, they fail to obtain the correct position of the d-bands. This leads, for instance, to the underestimation of the interband absorption onset in the corresponding optical spectra as shown for a set of elemental metals [1]. In this work, we provide a systematic investigation of the quasi-particle band structure and the optical properties of this set of materials. To this extent, the self-energy corrections to the DFT results are computed by the GW approach of many-body perturbation theory as implemented in the full-potential all-electron code exciting [2,3]. We show that the optical absorption spectra based on these quasi-particle bands remedy the shortcomings of semi-local DFT, accurately reproducing the experimental counterparts.

[1] W. S. M. Werner, K. Glantschnig, and C. Ambrosch-Draxl, J. Phys. Chem. Ref. Data 38, 1013 (2009). [2] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, J. Phys: Condens. Matter 26, 363202 (2014). [3] D. Nabok, A. Gulans, and C. Draxl, Phys. Rev. B 94, 035418 (2016).

O 35.7 Tue 12:30 TRE Ma

Separable Resolution-of-Identity in an all-electron numeric atom-centered basis set framework — •Francisco Delesma[1], Dorothea Golze[2], and Patrick Rinke[1] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Dresden, Germany

The resolution-of-identity (RI) is a common way in quantum chemistry and computational materials science to reduce the computational cost of two-electron Coulomb integrals, another central entity in computational quantum mechanics. In 2019, Duchemin and Blase proposed the separable-RI approach [1], which preserves the accuracy of the standard, global RI method with the Coulomb metric (RI-V) and permits the formulation of cubic-scaling random-phase approximation (RPA) and Green's function based GW approaches.

In this work, we present the first implementation of the separable-RI in an all-electron numeric atom-centered orbital framework. Separable-RI is implemented in the FHI-aims code [2] and optimized for massively parallel execution. We extend the separable-RI framework beyond the original Hartree-Fock (HF) and GW implementations of Duchemin and Blase to MP2 and RPA, SOSEX and CCSD. Our separable-RI total energies and GW quasiparticle energies for the Thiel test set of small organic molecules reproduce the exact two-electron Coulomb integral calculations within 1 meV or better.

[1] I. Duchemin and X. Blase, J. Chem. Phys. 150, 174120 (2019)
[2] V. Blum, et al, Comput. Phys. Commun. 180, 2175, (2009)

O 36: Poster: 2D Materials II

Time: Tuesday 18:00–20:00 Location: P2/EG

O 36.1 Tue 18:00 P2/EG

Simulation of proximity effects in epitaxial graphene systems — •Andres David Peña Unigarro[1], Florian Steffen Günther[2,3], and Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz, Chemnitz, Germany — [2]IFSC, University of São Paulo, Brazil — [3]UNESP, Brazil

Two-dimensional materials such as graphene are fascinating because they combine mechanical flexibility with unique electronic properties. The next level of complexity, however, comprises the assembly of various 2D materials to generate structures with enhanced characteristics. Using proximity effects, changes in the electronic, optical and transport properties of epitaxial graphene have been produced while preserving the regular honeycomb structure that can be grown on silicon carbide, SiC. Such modifications can, for instance, be achieved by proximity effects in hetero stacks with intercalate and absorbate layers with other 2D materials or by the presence of a functional integration environment. In the past years, many elements were intercalated below the graphene sheet, forming partly well-defined hetero bilayer systems with different functionalities. As suggested by density functional theory (DFT) studies, elements of the IV group can be used for this purpose. In this case, intercalation of heavy atoms like Pb are expected to introduce additional effects such as spin-orbit coupling to the electron gas of graphene. In this contribution, we present preliminary results obtained with DFT focusing on the study of modifications of the electronic structure of epitaxial graphene due to proximity effects generated by the intercalation of Pb on buffer layers on SiC.

O 36.2 Tue 18:00 P2/EG

Structural Characterization of a Novel Two-Dimensional Material: Cobalt Sulfide Sheets on Au(111) — •Marcel Rost[1], Mahesh Prabhu[2], Dajo Boden[2], Jörg Meyer[2], and Irene Groot[2] — [1]Huygens-Kamerlingh Onnes Laboratory, Leiden Institute of Physics, Leiden University, 2300 RA Leiden, The Netherlands — [2]Leiden Institute of Chemistry, Leiden University, P.O. Box 9502, 2300 RA Leiden, The Netherlands

Transition metal dichalcogenides (TMDCs) are a type of two-dimensional (2D) material that has been widely investigated by both experimentalists and theoreticians because of their unique properties. In the case of cobalt sulfide, density functional theory (DFT) calculations on free-standing S-Co-S sheets suggest there are no stable 2D cobalt sulfide polymorphs, whereas experimental observations clearly show TMDC-like structures on Au(111). In this study, we resolve this disagreement by using a combination of experimental techniques and DFT calculations, considering the substrate explicitly. We find a 2D CoS(0001)-like sheet on Au(111) that delivers excellent agreement between theory and experiment. Uniquely this sheet exhibits a metallic character, contrary to most TMDCs, and exists due to the stabilizing interactions with the Au(111) substrate.

O 36.3 Tue 18:00 P2/EG

Carbon Nanomembranes Fabricated from Amorphous Molecular Layers — •Zhen Yao[1], Nikolaus Meyerbröker[2], Yubo Qi[1], Michael Westphal[1], Yang Yang[1], and Armin Gölzhäuser[1] — [1]Bielefeld University, Bielefeld, Germany — [2]CNM Technologies, Bielefeld, Germany

Ultrathin carbon nanomembranes (CNMs), fabricated from crosslinking self-assemblies of molecular precursors, are 2D membranes that possess well-defined physical and chemical properties. With a simple transfer procedure, CNMs can be placed on various supports, enabling versatile applications. Combining high water flux and precise ion selectivity, CNMs are ideal materials for molecular separation and water desalination. However, their practical realization is hindered by the availability of epitaxial metal substrates. Here, we report a new type of CNM fabricated from poly(4-vinylbiphenyl) (PVBP) spin-coated on SiO2/Si substrate. The electron-induced crosslinking results in the formation of a continuous membrane with a thickness of 15 nm. The nanoporous nature of the PBVP-CNM is revealed by water and ion permeation measurements. The membrane possesses a high density of pores, which allows water flux as high as 530 L m-2 h-1 bar-1. It also exhibits the rejection of ions and molecules with sizes >1 nm. A further introduction of a reinforcement porous block copolymer layer simplifies the transfer procedure, resulting in a centimetre-scale CNM-composite that works efficiently for dye rejection. These results suggest a feasible route for large-scale nanoporous membrane fabrication.

O 36.4 Tue 18:00 P2/EG

A New Group of Two-Dimensional Non-van der Waals Materials with Ultra Low Exfoliation Energies — •Tom Barnowsky[1,2], Arkady V. Krasheninnikov[1,3], and Rico Friedrich[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Theoretical Chemistry, Technische Universität Dresden, 01062 Dresden, Germany — [3]Aalto University, Aalto 00076, Finland

The exfoliation energy, *i.e.* the energy required to separate a single two-dimensional (2D) sheet from a bulk material, is a key factor in whether such 2D systems can be made. Recently, non-van der Waals 2D compounds – materials derived from non-layered bulk counterparts – were outlined as a rich new class of nanoscale materials [1].

In our work, using data-filtering and ab-initio calculations, we propose a group of eight novel non-van der Waals 2D systems [2]. The compounds exhibit ultra-low exfoliation energies close to those of traditional van der Waals bound 2D materials. Especially for the considered sulfides, strong surface relaxations play a key role in the energy gain enabling exfoliation, while the effects of long-range dispersive interactions are minor. The candidates with the smallest exfoliation energies, 2D $SbTlO_3$ and $MnNaCl_3$, exhibit appealing electronic, potential topological, and magnetic features as evident from the calculated band structures.

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[2] T. Barnowsky *et al.*, submitted (2022).

O 36.5 Tue 18:00 P2/EG

Magnetic properties of transition metal dihalides measured by x-ray magnetic circular dichroism (XMCD) — •Sebastien Elie Hadjadj[1], Samuel Kerschbaumer[2], Andrea Aguirre Banos[3], Danilo Longo[3], Fadi Choueikani[4], Celia Rogero[2], Jose Ignacio Pascual[3], Wolfgang Kuch[1], and Maxim Ilyn[2] — [1]Institut für Experimentalphysik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Centro de Fisica de Materiales (CSIC/UPV-EHU), 20018 Donostia-San Sebastian, Spain — [3]CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastian, Spain — [4]Synchrotron SOLEIL, 91190 Saint-Aubin, France

During the last couple of years, there has been a rising interest in novel two-dimensional magnetic materials. Most recently, several groups have shown that magnetic order in two-dimensional materials can be stable [1]. Here we report the single phase epitaxial growth of ML to multilayer CoBr2 and CoCl2 Au(111) as well as on NbSe2. The samples where characterized via LEED, XPS, XAS, XMCD and LT-STM. Both Co-compounds show a strong in-plane anisotropy and ferromagnetic order up to temperatures of around 20 K.

[1] Djuro Bikaljevic et al., ACS Nano, 15, 14985 (2021)

O 36.6 Tue 18:00 P2/EG

Silicene's pervasive surface alloy on Ag(111) — Johannes T Küchle[1,2], Aleksandr Baklanov[1], Ari P Seitsonen[3,4], Paul TP Ryan[2,5], Peter Feulner[1], Prashanth Pendem[1], Tien-Lin Lee[2], Matthias Muntwiler[6], Martin Schwarz[1], Felix Haag[1], Johannes V Barth[1], Willi Auwärter[1], •David A Duncan[1,2], and Francesco Allegretti[1] — [1]Physics Department E20, Technische Universität München, Deutschland — [2]Diamond Light Source, Oxfordshire, UK — [3]Département de Chimie, École Normale Supérieure, Paris, France — [4]Université Paris Sciences et Lettres, Sorbonne Université, Paris, France — [5]Imperial College London, UK — [6]Paul Scherrer Institut, Villigen, Switzerland

Silicene is the two-dimensional (2D) allotrope of silicon. So far, the most direct synthesis strategy has been to grow it epitaxially on metal surfaces; however, the effect of the strong silicon-metal interaction on the structure and electronic properties of the metal-supported silicene is generally poorly understood. Here, we consider the (4×4)-silicene monolayer (ML) grown on Ag(111), and show that our experimental results refute the common interpretation of this system as a simple buckled, honeycomb ML with a sharp interface to the Ag substrate. Instead, we demonstrate the pervasive presence of a second silicon species, concluded to be a Si/Ag alloy stacked between the 2D silicene and the silver substrate. These findings question the current structural understanding of the silicene/Ag(111) interface and may raise expectations of analogous alloy systems in the stabilization of other 2D materials grown epitaxially on metal surfaces.

O 36.7 Tue 18:00 P2/EG

Pb-induced proximity effects in epitaxial graphene — Andres David Pena Unigarro, Chitran Ghosal, •Christoph Tegenkamp, and Sibylle Gemming — Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, 09126 Chemnitz

A current topic in material science deals with the controlled assembly of various 2D materials to generate structures with new quantum characteristics. Such modifications can be achieved by proximity effects, e.g., by intercalation and adsorption. One promising route is to use epitaxial buffer layer structures on SiC(0001) surfaces, which transforms into a quasi free monolayer graphene with new 2D interface structures upon intercalation. As suggested by density functional theory (DFT) studies, elements of the IV group such as Pb can be used for this purpose. In this case, intercalation of heavy atoms like Pb are expected to introduce additional effects such as spin-orbit coupling to the electron gas of graphene. In this contribution, we investigated the intercalation of Pb on buffer layers on SiC(0001). Suspended and charge neutral graphene emerged, and the intercalated Pb formed plumbene honeycomb lattices, which are rotated by 7.5° with respect to graphene. Along with this twist, a proximity-induced modulation of the hopping parameter in graphene opens a band gap of around 30 meV at the Fermi energy, giving rise to a metal-insulator transition. We present first results obtained with DFT focusing on the modifications of graphene's electronic structure in the presence of twisted Pb layers.

O 36.8 Tue 18:00 P2/EG

Local spectroscopy of acoustic phonons in low-dimensional materials — •Yi Zhang[1], Shaoxiang Sheng[1,2], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Coherent acoustic phonons (CAPs) enable ultrafast control of solids and have been exploited for applications in various acoustic devices. THz-induced ultrafast Coulomb forces in a scanning tunnelling microscope (STM) junction can locally generate CAP wave packets that propagate with low losses and form longitudinal acoustic standing waves in a thin Au film on mica [1,2]. Here we develop a discrete lattice model to simulate acoustic phonon propagation in well-defined nanostructures. We predict that transverse acoustic phonons can be detected in 1D chains or in 2D thin films by THz-STM. This enables investigation of mechanical properties and electron-phonon interaction in nano-materials at the atomic scale. [1] S. Sheng, et al. Physical Review Letters 129, 043001 (2022). [2] M. Abdo, et al. ACS Photonics 8, 702-708 (2021).

O 36.9 Tue 18:00 P2/EG

Structure and electronic properties of antimonene on Ag(111) — •Friedrich Wanierke, Felix Otto, Maximilian Schaal, Marco Grünwald, Lorenz Brill, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University jena, Helmholtzweg 5, 07743 Jena

The synthesis of new two-dimensional (2D) materials is of great interest for the development of new designs of electronic devices. In this study, we payed special emphasis on the growth of the elemental 2D semiconductor antimonene on Ag(111) by molecular beam epitaxy. To characterize and evaluate the deposited films, we used various methods of surface science. On the one hand, we performed in situ reflection high energy electron diffraction (RHEED), low energy electron diffraction (LEED) and low-temperature scanning tunneling microscopy (STM) for structural investigations. On the other hand, photoelectron spectroscopy as well as STM were used to reveal the electronic properties of the ultra-thin films. The alloy Ag_2Sb, as well as β- and α-antimonene, with respect to the amount of deposited antimon, are discussed.

O 36.10 Tue 18:00 P2/EG

Impact of screening and relaxation on weakly coupled 2D heterostructures: implications for molecular spin-coupling — Eva Rauls[1], T.T. Nhung Nguyen[2], Christoph Tegenkamp[2], and •Uwe Gerstmann[3] — [1]University of Stavanger, Norway — [2]Technische Universität Chemnitz, Germany — [3]Universität Paderborn, Germany

Phthalocyanines (Pc) at surfaces are prototype molecules which can host magnetic ions in a well-defined surface environment. The precise external control of individual spins, however, require a detailed knowledge of the influence of the substrate. In this combined experimental and theoretical study, we have investigated the influence of different graphene-related substrates onto the structural, electronic and magnetic properties of adsorbed Pb and Mn-phthalocyanines. Formation of almost identical densely packed PbPc molecular layers with strongly tilted molecules were found on *n*-type and *p*-type doped 2D templates. On graphite (HOPG), the dispersing molecular states of the less deformed molecular adsorbate stress the importance of substrate mediated interaction and proximity coupling [1]. After substituting Pb by magnetic Mn, the interaction with the substrate is clearly increased. On epitaxial monolayer graphene (MLG) the MnPc experience even the underlying SiC substrate, resulting in a 4×2 reconstructed molecular layer with very specific substrate mediated magnetic coupling.

[1] T.T. Nhung Nguyen, T. Sollfrank, C. Tegenkamp, E. Rauls, U. Gerstmann, Phys. Rev. B 103, L201408 (2021).

O 36.11 Tue 18:00 P2/EG

Honeycomb structure of alkali metal atoms — Jiaqi Cai[1,2,3], •Robin Ohmann[1], Nicolae Atodiresei[4], Hai Chau Nguyen[1], David Duncan[5], Caio Silva[2], Christoph Schlueter[5], Kai Mehlich[1], Thais Chagas[1], Vasile Caciuc[4], Wouter Jolie[3], Stefan Blügel[4], Tien-Lin Lee[5], Thomas Michely[3], and Carsten Busse[1,2,3] — [1]Department Physik, Universität Siegen, Siegen, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany — [3]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [4]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, Jülich, Germany — [5]Diamond Light Source, Didcot, Oxfordshire, United Kingdom

The formation of honeycomb structures, similar to graphene, is of great scientific and technological interest. Here, we show that the adsorption of Cs on monolayer hexagonal boron nitride (hBN) on Ir(111) substrate kept at elevated temperatures forms a honeycomb lattice. The structure is investigated by scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and X-ray standing waves (XSW) revealing that the Cs atoms are in registry with the moiré pattern of the substrate with a lattice constant of about 30 Å, are partially positively charged and have an adsorption height of 2.9 Å above the hBN layer. The formation is explained via the templating effect of the substrate. Our density functional theory (DFT) results confirm stable binding on the two hill regions of the moiré unit cell and predict a graphene like band structure with a band width of about 1 meV.

O 36.12 Tue 18:00 P2/EG

Unstrained Sb Bilayers on InSb(111)A — Bing Liu[1,2], •Stefan Enzner[1,3], Tim Wagner[1,2], Philipp Eck[1,3], Martin Kamp[2], Giorgio Sangiovanni[1,3], and Ralph Claessen[1,2] — [1]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany

Antimonene, a hexagonal arrangement of staggered Sb, is a promising topological material, which has been widely investigated on various substrates. Recently, it has been grown strain-free on InSb(111)A by forming a moiré structure, despite exhibiting covalent interface bonds.

The moiré supercell is theoretically approximated with varying interface stackings of primitive cells by means of ab initio DFT calculations. This approach reproduces the main structural and electronic observations. The agreement allowed us, to investigate the competition of intra-layer and interface interactions and explain the reconstruction-free growth.

O 37: Poster: Ultrafast Electron Dynamics at Surface and Interfaces II

Time: Tuesday 18:00–20:00 Location: P2/EG

O 37.1 Tue 18:00 P2/EG

Probing alternative pathways for electron transfer across a monomolecular film — Saunak Das[1], Zhiyong Zhao[1], Takanori Fukushima[2], Andreas Terfort[3], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Laboratory for Chemistry and Life Science, Institute of Innovative Research, Tokyo Institute of Technology, Yokohama 226-8503, Japan — [3]Institut für Anorganische und Analytische Chemie, Johann Wolfgang-Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

Charge transport (CT) across a two-dimensional molecular assembly can involve alternative pathways. Using specifically designed monomolecular films we probe (i) competition of intramolecular and intermolecular pathways in a molecular assembly and (ii) competition of different intramolecular pathways within a single molecule. For this purpose, we apply so-called core-hole-clock approach in the framework of resonant Auger electron spectroscopy, allowing the measurement of the characteristic CT time from the terminal tail group of the assembled molecules to the substrate. We show that the intramolecular CT is generally preferable and so-called matrix effects play a negligible role for CT, strongly favoring the through-bond CT model. In the case of availability of several alternative pathways within an individual molecule, a pathway with the highest conductance becomes highly dominant, while other pathways contribute minorly to the entire CT.

O 37.2 Tue 18:00 P2/EG

Pump-probe second harmonic spectroscopy of molecule/metal interfaces — Jinghao Chen[1], Rui Shi[2], Ping Zhou[1], Uwe Bovensiepen[1], Wolfgang Hübner[2], Georg Lefkidis[2], and •Andrea Eschenlohr[1] — [1]Faculty of Physics and CENIDE, Uni Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Department of Physics, TU Kaiserslautern, Box 3049, 67653 Kaiserslautern, Germany

Achieving a microscopic understanding of charge transfer dynamics and the relaxation of optically excited electrons and holes at molecule/metal interfaces requires an interface-sensitive analysis on the respective femtosecond timescales. Second harmonic spectroscopy (SHS) is such an interface-sensitive probe in centrosymmetric materials. We perform pump-probe SHS in the visible wavelength range (1.9-2.5 eV) with <20 fs pulse duration. A prototypical molecule/metal interface is prepared by adsorption of iron octaethylporphyrin (FeOEP) molecules on Cu(001) and analyzed *in situ* in ultrahigh vacuum. By comparison with first principles theory, we identify a molecule-induced resonance at about 2.2 eV fundamental photon energy in the SHS of one monolayer of FeOEP/Cu(001). At this resonance, we observe a markedly slower relaxation time of the pump-induced changes in SHS compared to the bare Cu(001) surface, which indicates an increased lifetime of the electronic molecular state.

We thank H. Wende, J. Güdde and E. Riedle for valuable experimental advice, and the German Research Foundation for funding via SPP 1840 QUTIF and Sfb 1242.

O 37.3 Tue 18:00 P2/EG

Second harmonic spectroscopy of Cu(001) surfaces — •Newsha Vesalimahmoud, Jinghao Chen, Mahendra Kabbinahithlu, Ping Zhou, Uwe Bovensiepen, and Andrea Eschenlohr — University of Duisburg-Essen, Faculty of Physics and CENIDE, Lotharstr. 1, 47057 Duisburg, Germany

The nonlinear optical technique of second harmonic generation (SHG) is a surface- and interface-sensitive tool in centrosymmetric materials, which is used to study electron dynamics at metal surfaces. We characterize the polarization and wavelength dependent SHG on a Cu(001) surface using a fundamental beam in the wavelength range of 500 - 700 nm. Polarization dependent measurements show the p-P SHG yield is almost a factor of 1.5 larger than s-P SHG, because more non-zero susceptibility tensor elements are involved in the former and the intrinsic absolute value of $|\chi^{(2)}_{zzz}|$ is much larger than the only relevant component $|\chi^{(2)}_{zxx}|$ in the latter. We also measure the spectral dependence of the SHG intensity, which shows an increase up to a maximum at 2.33 eV. Since the 3d band peak of copper lies about 2.3 eV below Fermi level, a fundamental beam at this photon energy can resonantly excite 3d electrons to the Fermi level, which largely increases the overall probability of SHG processes. Moreover, we discuss electron dynamics analyzed through pump-probe SHG at on and off-resonant photon energies.

O 37.4 Tue 18:00 P2/EG

Formation mechanism of defect levels 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 have been widely studied as TiO_2 is a prototypical photocatalyst. Recent studies have specifically addressed the Band Gap State (BGS) at 0.8 eV below the Fermi level and have revealed its role as a trapping center for electrons in the conduction band of rutile $TiO_2(110)$ (with a trapping time of around 45 fs) [1]. However, the origin of the BGS itself remains debated. Using time-resolved photoelectron spectroscopy, we show here that the BGS must be - at least partially - due to long-lived (>5 μs) photoexcited charge carriers which form a photostationary state in pump-probe experiments. The potential formation mechanism of the BGS and implications of this state for previous time-resolved experiments are discussed.

Reference:

[1] Zhang et al. J. Phys. Chem. Lett. 10(52) (2019).

O 37.5 Tue 18:00 P2/EG

Investigation of low-temperature electron emission properties from sharp needle tips — •Manuel Knauft, Stefan Meier, Norbert Schönenberger, and Peter Hommelhoff — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Spectroscopic and microscopic techniques benefit from the small linewidth of coherent electron sources with high brightness. Reducing the operating temperature of the emitter is known to positively influence coherence of field emitted electron beams. This is especially true for superconducting needle tips as shown for niobium [1].

We present an experimental setup capable of cooling electron emitters to liquid helium temperature in ultra-high vacuum. Irradiation of samples with ultrashort laser pulses is possible through optical access to the chamber. Detection of charged particles is realized by a multichannel plate. First results for sharp needle tips of various materials are shown. In particular, we investigate the emission characteristics and compare them for field emission and laser triggered emission as a function of temperature.

[1] Nagaoka *et al.*, Nature **396**, 557 (1998)

O 37.6 Tue 18:00 P2/EG

Magnetic field effects on ultrafast driven electrons in topological insulator surface states — •Alexander Riedel[1], Vanessa Junk[1], Wolfgang Hogger[1], Cosimo Gorini[2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Germany — [2]Universite Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

When strong-field light pulses of various durations and shapes interact with a solid, their electric field component acts as an a.c. bias accelerating electrons through the bandstructure and driving non perturbative transitions. These processes can lead to high-order harmonic emission of radiation which encodes characteristic properties of the underlying material.

However, in the vast majority of cases the magnetic field component of the pulse is completely neglected in theoretical descriptions. In this contribution we incorporate a magnetic field into the description by adding a Zeeman term into an effective minimal model Hamiltonian describing the surface states of the topological insulator material bismuth telluride. We present how magnetic field components influence the Berry curvature and the transitions induced by the pulse. The resulting currents and higher harmonic spectra are discussed and compared to those in the absence of magnetic field effects. All statements rely on both a semiclassical analysis and full quantum mechanical simulations.

O 37.7 Tue 18:00 P2/EG

Use cases for Picosecond Ultrasonics with X-rays (PUX) — •Alexander von Reppert[1], Maximilian Mattern[1], Steffen Zeuschner[1,2], Jan-Etienne Pudell[1,2,3], Marc Herzog[1], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität 14476 Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum Berlin, 12489 Berlin, Germany — [3]European XFEL, 22869 Schenefeld, Germany

Most studies of picosecond ultrasound have been and will be conducted with flexible all-optical setups, but here we discuss scenarios where ultrashort hard x-ray probe pulses excel. We focus on the extraction of the strain response from Bragg peak shifts in the symmetric diffraction condition for layered, nanoscopic structures upon excitation of metallic transducers with femtosecond laser pulses. This type of experiment can yield direct, layer-specific and quantitative information on the shape and amplitude of picosecond strain pulses and the quasi-static strain. The strain response may serve as a proxy for the local energy-density and temperature rise. The presented use-cases encompass ultrahin as well as opaque metal-heterostructures, nanostructures and negative thermal expansion materials, that each pose a challenge to established all-optical techniques.

O 37.8 Tue 18:00 P2/EG

Photocatalysis on anataseTiO2(101) in real-time — •Heshmat Noei[1,2], Michael Wagstaffe[1], Adrian Dominguez-Castro[3], Lukas Wenthaus[1], Steffen Palutke[1], Dmytro Kutnyakhov[1], Michael Heber[1], Federico Pressacco[1], Sirhei Dziarzhytski[1], Helena Gleissner[1], Verena Kristin Gupta[1], Adriel Dominguez[1], Thomas Frauenheim[3], Angel Rubio[4], and Andreas Stierle[1] — [1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [3]Bremen Center for Computational Material Science (BCCMS), D-28359, Bremen, Germany — [4]Max Planck Institute for the Structure and Dynamics of Matter, D-22761, Hamburg, Germany

Obtaining mechanistic insight surrounding interfacial charge transfer and the role of intermediate species during photocatalysis on metal oxide surfaces is challenging due to their ultrafast nature. By applying ultra-fast optical pump-soft X-ray probe experiments at FLASH in DESY, we have obtained first insight into the activation mechanism of CO photooxidation to CO2 on rutile and anatase TiO2 surfaces and charge transfer at the interfacxe of water and TiO2(101). By using an optical laser of 800 nm and a FEL energy of 647.8 eV, the changes in the Ti 2p, O 1s and C 1s core levels have been monitored on a picosecond timescale.

O 37.9 Tue 18:00 P2/EG

Ultrafast UV pulse generation at the SXP instrument of the European XFEL — •Ekaterina Tikhodeeva[1], Patrik Grychtol[1], Marcus Seidel[2], Christoph M. Heyl[2], Vahagn Vardanyan[1], David Doblas-Jimenez[1], and Manuel Izquierdo[1] — [1]European XFEL, Schenefeld, Germany — [2]DESY, Hamburg, Germany

At the European XFEL a new instrument, the Soft X-ray Port (SXP), is currently under commissioning. Located downstream of the SASE 3 soft X-ray undulator system, it will provide femtosecond photon pulses with variable polarization in the energy range between 260 eV and 3000 eV at MHz repetition rates. Up to 10^{12} photons per pulse will be focus at the interaction region in a micrometer spot size resulting in an intensity of more than 10^{18} W/cm^2. The energy range will enable the complete electronical, chemical and atomic characterization of solids, surfaces and interfaces using femtosecond time-resolved soft X-ray photo-electron spectroscopy. Moreover, two powerful pump lasers operating in a broad spectral range from the mid-infrared to the ultraviolet region will be available. Herriott multi-pass cells (HMPC) will be used to compress their pulses into the few femtosecond range paving the way for ultrafast pump-probe investigations at the SXP instrument combining intense and tunable soft X-rays with the versatile optical lasers. In this contribution, the development of the HMCP and the optical laser system will be presented.

O 37.10 Tue 18:00 P2/EG

Transferring photonic orbital angular momentum to metals — •Jannis Lessmeister[1], Tobias Eul[1], Eva Prinz[1], Sebastian Hedwig[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, Germany

Optical fields can carry an orbital angular momentum (OAM) in helical beams with an azimuthal phase dependence. Since the discovery of this phenomenon in 1992 [1], the interaction of photonic OAM with matter has become a steadily growing field of research. After an initial focus on atoms and molecules, in the last years, scientists also began investigating solids [2]. For example, recent studies revealed that the so-called twisted light can drive photocurrents [3] and affects ultrafast demagnetization dynamics [4].

In our research, we apply time- and angle-resolved photoelectron spectroscopy (TR-ARPES) to gain new insight into the influence of photonic OAM on the hot carrier dynamics in metals. Specifically, we investigated the influence of the added orbital angular momentum on the optical excitation efficency of photoelectrons from the spin-split band structure of Rashba surface states and the hot carrier dynamics of spin-dependent carriers in the ferromagnet Ni.

[1] Allen et al., Phys. Rev. A 45 (1992)
[2] Quinteiro Rosen et al., Rev. Mod. Phys 94 (2022)
[3] Ji et al., Science 368 (2020)
[4] Prinz et al., arXiv:2206.070502 (2022)

O 37.11 Tue 18:00 P2/EG

Combining THz-ARPES and THz-HHG to study electrical currents at buried interfaces of topological insulators — •Tim Bergmeier, Suguru Ito, Jens Güdde, and Ulrich Höfer — Fachbereich Physik, Philipps-UniversitätMarburg, Germany

Angle-resolved photoemission spectroscopy (ARPES) combined with terahertz (THz) excitation has shown to provide a subcycle-resolved momentum space view of lightwave-driven Dirac currents in the surface band of topological insulators [1]. At high electric field strength, these currents have shown to give rise to a unique type of efficient high-harmonic generation (HHG) that reflects the unusual transport properties of the Dirac electrons [2]. As a pure optical technique, THz-HHG is able to access also deeply buried interfaces, but lacks band structure information.

Here, we present an experimental setup which combines both techniques in order to study first the impact of thin protection layers on the current transport in a topologically protected band. The correlation of the time-resolved band structure information provided by THz-ARPES with the properties of THz-HHG will then allow us to apply the latter for thick layers as will be required for device applications. The setup includes the generation of THz-pulses with field strengths up to 10 MV/cm over a frequency range of 12-80 THz, and of ultrashort 400-nm probe pulses for two-photon photoemission with subcycle time resolution at a repetition rate of 200 kHz.

[1] J. Reimann *et al.*, Nature 562, 396 (2018).
[2] C. P. Schmid *et al.*, Nature 593, 385 (2021).

O 37.12 Tue 18:00 P2/EG

A narrow bandwidth extreme ultra-violet light source for time- and angle-resolved photoemission spectroscopy — Qinda Guo[1], Maciej Dendzik[1], Antonija Grubišić-Čabo[1], Magnus H. Berntsen[1], Cong Li[1], •Wanyu Chen[1], Bharti Matta[2], Ulrich Starke[2], Björn Hessmo[1], Jonas Weissenrieder[1], and Oscar Tjernberg[1] — [1]Department of Applied Physics, KTH Royal Institute of Technology, Hannes Alfvéns väg 12, 114 19 Stockholm, Sweden — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Here, we present a high repetition rate, narrow bandwidth, extreme ultraviolet photon source for time- and angle-resolved photoemission spectroscopy. The narrow bandwidth pulses ΔE = 9, 14, and 18 meV for photon energies hν = 10.8, 18.1, and 25.3 eV are generated through high harmonic generation using ultra-violet drive pulses with relatively long pulse lengths (461 fs). The high harmonic generation setup employs an annular drive beam in tight focusing geometry at a repetition rate of 250 kHz. Photon energy selection is achieved by a spherical focusing grating, which provides high efficiency photon flux with only a small amount of focus size increase (˜30%) and temporal broadening (6.8%). A two stage optical-parametric amplifier provides < 100 fs tunable pump pulses from 0.65 μm to 9 μm. Combined with a time-of-flight electron analyzer, the setup enables for high-resolution studies of ultrafast dynamics over the whole surface Brillouin zone in most quantum materials.

O 37.13 Tue 18:00 P2/EG

Time Resolved Photoelectron Spectroscopy of Thiophen based Conjugated Donor Aceptor Polymers for Organic Photovoltaic — •Tobias Reiker[1], Pradny Phanse[1], Nils Fabian Kleimeier[1], Zitong Liu[2], Adrian Urban[1], Deqing Zhang[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, University of Münster, Germany — [2]Institute of Chemistry, Chinese Academy of Science, Beijing, China

Thiophene-based polymers are promising candidates for solar cell, OLED or transistor applications. An internal donor - acceptor system is formed by coupling thiophene polymers with pyrrole chains. We report results of temporally resolved photoemission studies on thiophene polymers on silicon substrates. The charge transport behaviour can be tuned by different alkyl side chains since they influence the electronic structure and aggregation. A direct assessment of the intramolecular and intermolecular dynamics may guide synthesis routes. With pF8T2, pDPP4T, pDPP4T-1 and pDPTTT we investigated the electronic dynamics of high hole-mobility organic semiconductors. Either the backbone or the side chains were modified. With the blend of pDPP4T-1 and a Fullerene we compare the excitation dynamics of singe component und blended OPV. These different molecular configurations are intended to provide insights into the change in electron configuration due to both backbone modification and intermolecular packing.

O 38: Poster: Organic Molecules on Inorganic Substrates II

Time: Tuesday 18:00–20:00 Location: P2/EG

O 38.1 Tue 18:00 P2/EG

Engineering two-dimensional metal-organic networks on ferromagnetic surfaces — •Martin Anstett[1], Lu Lyu[1], Ka Man Yu[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Two-dimensional metal-organic networks (MONs) on noble-metal surfaces have been identified as versatile nanoarchitecture to manipulate electronic and magnetic properties at surfaces. In this contribution, we discuss the growth and the structure formation of a Co-T4PT network on epitaxial Co films grown on an Au(111) single crystal. Using scanning tunnelling microscopy, we will show that the T4PT molecules can coordinate with native Co adatoms forming a long-range ordered two-dimensional porous network structure. This network can further act as a decoupling and templating layer for the subsequent growth of C60 guest molecules. For a C60 sub-monolayer, we find that the periodicity of the network structure mainly determines the adsorption configurations of isolated C60 molecules while the structural properties of ordered C60 islands on the Co-T4PT network are substantially influenced by the intermolecular interaction between the C60 molecules. The findings show that the MON system can be a very flexible template to tailor the interfacial properties of molecular assemblies for molecular-based spintronics and electronics.

O 38.2 Tue 18:00 P2/EG

Film growth and stabilty of the Ionic Liquid [C_1C_1Im][Tf_2N] on Pt(111) — •Timo Talwar, Stephen Massicot, Afra Gezmis, Cynthia Fernández, Leonhard Winter, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie 2, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Solid catalyst with Ionic Liquid Layer (SCILL) is a new catalytic concept using the advantageous properties of Ionic Liquids (ILs) to improve the catalytic performance such as selectivity and long-term stability of a solid catalyst by the coated IL. In this context, extensive knowledge about the IL-metal interface properties is highly desired.

In this study, the growth and thermal behavior of ultrathin films of 1,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide [C_1C_1Im][Tf_2N] on Pt(111) are investigated under UHV conditions. The films are prepared in vacuum by physical vapor deposition and measured by angle-resolved and temperature-programmed X-ray photoelectron spectroscopy. Complementary information is gained by Scanning Tunneling Microscopy. At 200 K, an intact closed wetting layer can be deposited on Pt(111). The underlying growth mode is 2D up to 0.5 ML (a closed wetting layer) and moderate 3D for higher coverages. At higher temperatures up to 360 K, the IL continuously decomposes leading to desorption of volatile decomposition products. We will compare this behavior to previous results for this IL on the less-reactive Cu(111) and on the non-reactive Au(111) surface.

We acknowledge support by the DFG (SFB 1452 CLINT).

O 38.3 Tue 18:00 P2/EG

Thiahelicene non-covalent molecular wires on Cu(111) — •Gema Navarro[1], Antoine Hinaut[1], Shuyu Huang[1], Thilo Glatzel[1], Akimitsu Narita[2], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland. — [2]Okinawa Institute of Science and Technology Graduate University, Okinawa 904-0495, Japan

In recent years molecular nanowires have attained a paramount interest due to their potential application in the next generation of nanodevice. Therefore, researchers have been focused in the development of novel synthetic routes to achieve stable nanowires, also in the influence of heteroatoms doping to control optical or electronic properties [1]. Usually, the on-surface synthesis approach is adopted due to the robustness and versatile chemistry reactions available [2].

In the present study, we explore the deposition of thiahelicene molecules on Cu(111) as possible candidates for nanowires formation. Sample preparation and measurements were carried out at room temperature in an UHV system and the images were acquired by a noncontact AFM microscope. AFM-micrographic images illustrated the formation of molecular wires along the monocrystalline terraces. The growth process of the molecular wires retains the three-fold symmetry of the substrate, although, some defect points can be distinguished in their structure. In addition, the high mobility of the molecules indicates a weakly interaction with the copper surface.

[1] B. Mallada et al., ACS Appl. Mater. Interfaces 13, 32393 (2021).

[2] D.Y. Li et al., J. Am. Chem. Soc. 143, 12955 (2021).

O 38.4 Tue 18:00 P2/EG

Fabrication of Kondo Lattice via On-surface Reactions — •Jung-Ching Liu[1], Rémy Pawlak[1], Xing Wang[2], Chao Li[1], Outhmane Chahib[1], Ping Zhou[2], Robert Häner[2], Silvio Decurtins[2], Ulrich Aschauer[2], Shi-Xia Liu[2], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel — [2]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012 Bern

Magnetic atoms assembled in different lattices can exhibit various characteristics, such as spin frustration, heavy fermion, or spin textures via RKKY interaction[1]. Different from scanning probe tip manipulation[2] or e-beam evaporation[3], we perform on-surface reaction to realize magnetic lattice using pyrene-4,5,9,10-tetraone (PTO) and Fe on Ag(111)[4]. The STM and AFM structural investigation at 4K shows 1:1 coordination of PTO and Fe, resulting in 1D chains which further self-assemble into the close-packed pattern. Tunneling spectra measured at 1K confirm Kondo resonance localized on Fe atoms, with moderate dispersion on PTO. The dip lineshape of the Kondo resonance could indicate the spin-1 state on Fe[5]. The successful synthesis of magnetic organometallic structures demonstrates the tunability of Kondo lattice structure by changing molecule species. We believe our work enables fundamental studies of spin-spin and spin-substrate interactions with different spin lattices.[1] Moro-Lagares et al. Nat. Comm. 10, 2211 (2019)[2]Nadj-Perge et al. Science 346[3]Palacio-Morales et al. Sci. Adv. 5, eaav6600 (2019)[4]Pia et al. Chem. Eur. J. 22, 8105-8112 (2016)[5]Li et al. Chem. Commun. 54, 9135-9138 (2018)

O 38.5 Tue 18:00 P2/EG

Growth and structure of *p*-6P thin films as templates for organic heterosystems - a LEEM/PEEM study — •Franz Niklas Knoop, Winfried Daum, and Klaus Stallberg — Institute of Energy Research and Physical Technologies, TU Clausthal, Germany

The charge carrier dynamics at the contact of two organic semiconductors are strongly influenced by the molecular and mesoscopic structure of the interface. A systematic study of such structure-related effects on the carrier dynamics requires well defined and controllable model systems. Single-crystalline metals are suitable substrates for the epitaxial growth of well-ordered organic layers, but the carrier dynamics are strongly modified by the presence of a conductive surface. Therefore, we explore a different approach for the formation of organic/organic model systems: rod-like molecules such as parasexiphenyl (*p*-6P) are known to form highly ordered layers on weakly interacting amorphous substrates like SiO_2. These layers are suitable templates for the consecutive epitaxial growth of organic heterostructures. By thermal evaporation under ultrahigh vacuum conditions we deposit *p*-6P films with nominal mono- and bilayer thicknesses on natively oxidized silicon. Characterization with low-energy electron microscopy (LEEM) and atomic force microscopy (AFM) reveals coherent films which comprise single crystalline domains of upright-standing molecules. We discuss the influence of different growth parameters on the film structure and present results from two-photon photoemission electron microscopy (2P-PEEM). Moreover, first results from experiments with organic/organic heterosystems are also presented.

O 38.6 Tue 18:00 P2/EG

Understanding the role of adsorbed CTAB in anisotropic nanostructure growth — •Esmée Berger[1], Narjes Khosravian[1], Joakim Löfgren[2], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Department of Applied Physics, Aalto University, Espoo, Finland

A crucial step towards improved control over the shapes and sizes of wet-chemically synthesized nanostructures is a detailed theoretical understanding of the growth mechanism's different aspects. One of these aspects is the adsorption of surfactants, for example cetyltrimethylammonium bromide (CTAB), which is commonly used for structural tuning and increased stability. In water, CTAB exhibits a complex phase diagram, with a number of different liquid crystal-like phases. The complexity of the system is further increased during nanostructure growth, due to the presence of surfaces. Recent studies have indicated that the micellar phase of CTAB is the primary mechanism for anisotropic growth of silica and gold nanoparticles. These results were, however, based on a single value of the CTAB surface density. To properly understand the role of CTAB during anisotropic growth of nanostructures, a surface phase diagram must be established. In this work, we develop an understanding of the surface phase diagram from a modeling perspective, by means of molecular dynamics simulations.

O 38.7 Tue 18:00 P2/EG

Implementation of a silicon wafer into an UHV STM system for low temperature molecular depositions — •Ken Kolar, Grant Simpson, Christophe Nacci, and Leonhard Grill — Uni Graz, Graz, Austria

Sublimation temperatures of organic molecules typically rise as the number of constituting atoms is increased. This can lead to fragmentation and other experimental difficulties during molecular deposition if a standard sublimation Knudsen cell is used. One of the possibilities to overcome this problem is the deposition of molecules using the ”energy sudden” sublimation from a silicon wafer. We have installed such a system in our ultrahigh vacuum chamber and used it for depositions onto the sample that is kept at cryogenic temperatures during the preparation. Here, we present how such a device was implemented in our setup, together with first scannning tunneling microscopy (STM) images of the test depositions.

O 39: Poster Session: Heterogeneous Catalysis and Surface Dynamics

Time: Tuesday 18:00–20:00 Location: P2/EG

O 39.1 Tue 18:00 P2/EG

SURMOF ZIF-67 Thin Films for Catalytic Water Oxidation Reaction — •Jimin Song, Alexei Nefedov, Stefan Heissler, Christof Wöll, and Yuemin Wang — Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany

Metal-organic frameworks emerged as promising electrocatalysts to tackle urgent energy and environmental problems. Surface-coordinated MOF thin films (SURMOFs) were grown via a liquid phase epitaxial layer-by-layer method, endowed with precisely controlled thickness, preferred growth orientation and highly-ordered surface. For the first time, high-quality crystalline ZIF-67 SURMOF thin films were fabricated and employed in water oxidation reaction (OER). The transformation from ZIF-67 to CoOOH was observed after the water oxidation reaction by applying IRRAS, Raman and XPS measurements. Meantime, the thickness of the thin film decreased from 100 nm to 20 nm. The overpotential was reduced from 468 to 375 mA/cm2 by doping with boron and nickel.

O 39.2 Tue 18:00 P2/EG

SFG microscopy of ferroelectric domains in Barium Titanate — •Dorothee Mader[1], Daniel Lourens[2], Maarten Kwaaitaal[2], Richarda Niemann[1], Sören Wasserroth[1], Sandy Gewinner[1], Marco De Pas[1], Wieland Schöllkopf[1], Martin Wolf[1], Andrei Kirilyuk[2], Sebastian Maehrlein[1], and Alexander Paarmann[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Radboud Universiteit, Nijmegen, The Netherlands

Phonons exhibit a mostly unexplored leverage on ferroic order and its dynamics. Exploring the possibility of phonon-driven changes to the ferroelectric order provides an attractive route for potential applications of ferroelectric devices. Here, infrared-visible (IR-VIS) sumfrequency generation (SFG) microscopy with IR-sub-wavelength resolution [1] is employed combining resonant phonon excitation and ferroelectric domain imaging of barium titanate [BTO]. BTO is a noncentrosymmetric perovskite oxide with a strong ferroelectric polarization in its tetragonal phase at room temperature.Typically, BTO samples exhibit a multi-domain structure. Using the FHI Infrared (IR) free electron laser (FEL) in the range of 400-800 cm^{-1} different phonon modes of BTO are accessible. After characterization of the samples using linear optical techniques like polarization microscopy and infrared spectroscopy, the nonlinear optical properties of the ferroelectric domains are investigated using SFG-microscopy. By mapping phonon resonances in domains and domain walls, this approach may enable in-depth understanding of the underlying physics of domain formation. [1] R. Niemann et al., Appl. Phys. Lett. 120, 131102 (2022).

O 39.3 Tue 18:00 P2/EG

Investigating Heterogeneous Catalysts by Design of Experiments — •Christian Kunkel, Frederic Felsen, Sina Stocker, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

Bringing new and improved heterogeneous catalysts to market can be economically and ecologically rewarding. Yet, catalyst development is tedious, as a plethora of experimental factors in synthesis, formation and operation potentially influence achievable educt conversion and/or product selectivity. In the planning phase of an investigation, such influences can often only inadequately be assessed based on literature knowledge, individual experience and chemical intuition, resulting in a too narrow scope of experimentation. Data-driven approaches are less biased, potentially offering a way out. Still, the amount of recordable experimental data remains to be a limiting factor even with modern (automated) multi-reactor setups, where only a few dozen data points are acquired in reasonable time. In this contribution we therefore illustrate the practical application of highly-efficient optimally designed experiments. Leveraging simultaneous factor-changes, these jointly extract a maximum of information from each experimental run. Using examples from our ongoing investigation of thin-film and powder catalysts, we illustrate how this approach leads to significant insights on catalytic behavior over a larger number of factors. With additional information coming from multiple characterization techniques, we also demonstrate how catalyst development can strongly benefit from jointly coordinated data-driven experimental efforts.

O 39.4 Tue 18:00 P2/EG

Operando sXRD study of copper-zinc-alumina (CZA) model systems under methanol synthesis conditions — •Erik Beck[1,2], Vedran Vonk[1,2], Heshmat Noei[1,2], and Andreas Stierle[1,2] — [1]Centre for X-ray and Nano Science, Hamburg, Germany — [2]German Electron Synchrotron DESY, Hamburg, Germany

Methanol synthesis from gas mixtures of H2, CO and CO2 is an important industrial process in which copper-zinc-alumina (CZA) has been identified as a high performing catalyst. Typically, the products and reactants are gases used at pressures of >30 bar and a temperature of 250-300 degree C. Because of the dynamic nature of the catalyst under such industrial conditions, the underlying mechanisms and reaction paths are still under debate, since the traditional surface science techniques cannot be used at such high pressures. In order to bridge this pressure gap and gather structural information of the system in real operando conditions, we designed a special experimental setup for synchrotron-based high pressure SXRD. By using dedicated Cu and Zn UHV MBE growth chambers, we were able to prepare epitaxial model systems of the CZA catalysts composed of epitaxial Cu nanoparticles on Al2O3 single crystal surfaces. We performed operando high energy x-ray diffraction experiments on such model catalysts at up to 30 bar and 300degC at the High Energy Materials Science Beamline at DESY and we were able to follow the structural changes of the Cu nanoparticles during oxidation and reduction in different gas compositions.

O 39.5 Tue 18:00 P2/EG

Surface phase transitions in doped manganite thin films — •Leonard Schüler, Tim Titze, Stefan Mathias, Daniel Steil, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August-Universität Göttingen

The symmetry breaking at the surface of strongly correlated $La_{1-x}Sr_xMnO_3$ (LSMO) thin films leads to a modification of orbital occupation compared to the bulk resulting in the formation of intrinsic magnetic and electric surface phases. To obtain a phase diagram of possible surface states, LSMO films with Sr doping over the complete range $x = 0 - 1$ were prepared by metalorganic aerosol deposition and have been investigated by both surface-enhanced Raman spectroscopy (SERS) and pump-probe optical (SE-PPR) reflectivity. Temperature-dependent SERS reveals magnetic phase transitions by anomalous frequency shifts of the MnO_6 octahedra's stretching mode resulting from spin-phonon coupling, as well as changes in Mn orbital occupation inferred by enhanced Raman activity of vibrational Jahn-Teller modes at the surface. Furthermore, ultrafast dynamics studied by SE-PPR reveals a surface phase transition, which is not present in the bulk LSMO.

O 39.6 Tue 18:00 P2/EG

Laser pump X-ray probe investigations of the dynamics at the liquid-vapour interface of alkali halogenide salt solutions — •Lukas Petersdorf[1], Svenja Hövelmann[1,2], Rajendra Giri[1], Nicolas Hayen[1], Karin Hansen[1], Philipp Jordt[1], Andrea Sartori[1], Matthias Greve[1], Florian Bertram[2], Olaf Magnussen[1], and Bridget Murphy[1,3] — [1]University of Kiel (IEAP), Kiel — [2]DESY, Hamburg — [3]RHL, Kiel

Detailed knowledge of the surface of alkali halogenide solutions is fundamental for understanding atmospheric effects and developing technological applications such as solar thermal cells. Surface dynamics of such systems ranging from fs to s, can be studied in detail by pump-probe techniques. Our Laser pump-X-ray probe studies are based on photoionization processes at the interface induced by a 258 nm laser pulse and pumping electron solvation dynamics and ion rearrangements. With auspicious quantum yield and surface structure, the pump-probe studies were performed on salt solutions (NaI, RbBr, ErCl3). We apply the surface sensitive techniques time resolved XRR and GIXRF to investigate the responding structural changes. A sensor monitored sample environment allows us to distinguish between laser induced and solution dependent dynamics. Upon laser excitation, changes in the specular reflectivity occur on the ms to s scale. Electron density and surface roughness change near the interface indicate a rearrangement of the ion concentration. Within the framework of the DAPHNE4NFDI project, the analysis will be supported by artificial neural networks in order to allow in-operando experimental decisions.

O 40: Poster: Semiconductor Substrates

Time: Tuesday 18:00–20:00 Location: P2/EG

O 40.1 Tue 18:00 P2/EG

Si(553)-Au and Si(775)-Au surface reconstructions with a genetic algorithm approach — •Leonard M. Verhoff and Simone Sanna — Instutute for theoretical physics, Giessen, Germany

It was found by simulations and experiments, that Au atoms on a Si(553)- and Si(755)-surface form metallic nanowires. However, their precise atomic structure is still under discussion.

In this work, the respective surface reconstructions with N adatoms are searched, using a genetic algorithm implemented in the program *CALYPSO*. Genetic algorithms are reported to be efficient methods for structure predictions.

In the first generation, all Au atoms are distributed randomly on the surface, meaning every adatom introduces 3 degrees of freedom. For each generated structure, the fitness, i.e. the configuration's free energy, is then calculated from first principles with density functional theory implemented in *VASP*.

The next generation's individuals are created by moving every structure in the $3N$-dimensional space towards the structure that minimizes the fitness so far. To avoid getting stuck in a local energy minimum, 20% of the structured are created randomly in each generation.

The last step is repeated, until a certain convergence criterion is reached.

O 40.2 Tue 18:00 P2/EG

Assessing and processing the surface quality of free-standing wurtzite GaN in ultra-high vacuum — •Mohammadreza Rostami[1], Biao Yang[1], Felix Haag[1], Francesco Allegretti[1], Lifeng Chi[2], Martin Stutzmann[3], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, Garching, 85748, Germany — [2]Institute of Functional Nano & Soft Materials, Collaborative Innovation Center of Suzhou Nano Science and Technology, Soochow University, Suzhou 215123, P. R. China — [3]Walter Schottky Institute and Physics Department, Technical University of Munich, 85748 Garching, Germany

Gallium nitride (GaN) is proposed as an alternative candidate to metallic substrates for assembling organic molecular structures 1. However, the formation of a persistent surface oxide layer in air considerably limits the use of GaN for well-defined interfaces 1. We have investigated n-type free-standing c-plane wurtzite GaN crystals. The effect of electron bombardment on the surface quality of free-standing GaN during ammonia annealing was studied. Surface cleaning and full removal of the oxide layer on GaN surfaces could be reproducibly achieved via sputtering and annealing cycles, leading to substantial roughening of the GaN surface. Although ammonia annealing with electron bombardment increased the N/Ga atoms ratio, the surface morphology remained rough. In addition, the on-surface chemistry of 1,3,5-Tris(4-bromophenyl) benzene (TBB) 2 was studied on the cleaned GaN surface. [1] V. Bermudez, Surf. Sci. Rep. 72 (4), 147-315 (2017) [2] M. Fritton et al. J. Am. Chem. Soc 141 (12), 4824-4832 (2019)

O 40.3 Tue 18:00 P2/EG

A super-cycle approach to atomic layer deposition of indium-gallium-zinc oxide at low temperature — Ali Mahmoodinezhad[1], Carlos Morales[1], Małgorzata Kot[1], Franziska Naumann[2], Paul Plate[2], •Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]SENTECH Instruments GmbH, Berlin, Germany

The continuing development of multifunctional devices needs novel multicomponent oxide layers, demanding a high control of both composition and thickness during their preparation. To this end, single metal oxides exhibiting high structural quality and conformity have successfully been grown by atomic layer deposition (ALD). However, the deposition of more complex compounds with specific optical and electrical properties is still challenging. In this work, we follow a bottom-up approach to design an ALD super-cycle to grow mixed indium-gallium-zinc oxide (IGZO) films with a controllable composition. For the formation of the individual indium, gallium, and zinc oxides, we found the use of plasma-enhanced ALD (PEALD) at 150 °C to be favorable when using the organometallic precursors trimethylindium, trimethylgallium, and diethylzinc together with oxygen plasma. The PEALD approach of IGZO films can particularly overcome a nucleation delay within the ZnO sub-cycle known from thermal ALD, achieving a higher growth per cycle and improving the quality and composition homogeneity of the films as shown by in-situ spectroscopic ellipsometry and ex-situ X-ray photoelectron spectroscopy.

O 40.4 Tue 18:00 P2/EG

Adsorption of spike amino acids, asparagine and cysteine, on the surface of model catalyst TiO2 — •Miguel Blanco Garcia[1], Mona Kohantorabi[1], Michael Wagstaffe[1], Mohammad Tehrani[1], Silvan Dolling[1], Andreas Stierle[1,2], and Heshmat Noei[1] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [2]Mathematics, Informatics, and Natural Sciences (MIN) Faculty, University of Hamburg, 20354 Hamburg, Germany

Titanium oxides are excellent candidates for the inactivation of viruses using light due to their photocatalytic properties [1]. In this study we are aiming to determine the mechanism of inactivation of SARS-CoV-2 on TiO2 under ultraviolet treatment [2]. The two most abundant amino acids in the spike protein of the SARS-CoV-2 virus (cysteine and asparagine) [3] are adsorb under UHV and aqueous solution on TiO2 surfaces. Surface sensitive techniques such as X-ray photoelectron spectroscopy shows changes in the amino acids upon UV treatment. Furthermore, scanning tunneling microscopy demonstrates the disposition of the amino acid molecules on the surface and the changes upon UV irradiation. GISAXS data was obtain at DESY P03 for the adsorption in aqueous solution, to understand the adsorption geometry and self-assembly of the cysteine amino acids on the rutile and anatase TiO2 surfaces.

References: [1] Diebold, U. Surface science reports 48.5 (2003): 53-229. [2] Kohantorabi, et al., ACS Appl. Mater. Interface., Under Review. [3] Wang D, et al., Nano today 40 (2021): 101243.

O 41: Poster: Supported Nanoclusters

Time: Tuesday 18:00–20:00 Location: P2/EG

O 41.1 Tue 18:00 P2/EG

Nano-SMSI - FePt clusters on graphene/Rh(111) — •Natalie J. Waleska[1], Eva Marie Freiberger[1], Felix Hemauer[1], Valentin Schwaab[1], and Christian Papp[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Freie Universität Berlin, Germany

Strong metal-support interaction is found for particles supported on particular metal oxide surfaces leading, inter alia, to the encapsulation of the particle by a thin layer of the metal oxide support. As a result the adsorption ability is decreased strongly but also specific site blocking is found, offering new opportunities for site selective reactions.

In this work, we investigated graphene-supported FePt clusters on the Rh(111) single crystal surface by in situ high-resolution XPS and the utilization of CO as a probe molecule. The FePt clusters were prepared by successively depositing Fe (1.27 ML) and Pt (0.14 ML) on the graphene/Rh(111) substrate. Oxidation of Fe was achieved by beam induced CO dissociation. Heating of the FePt/graphene/Rh(111) sample to 550 K results in cluster ripening and the encapsulation of Pt by a thin FeO layer due to SMSI. Further increase of the temperature to 900 K, leads to the decomposition of the Fe oxide layer and the intercalation of Fe. Additionally the formation of a FePt alloy was observed at elevated temperature.

We thank Helmholtz-Zentrum Berlin for allocation of synchrotron-radiation beamtime and BESSY II staff for support during beamtime. This work was funded by the DFG within SFB 953 "Synthetic Carbon Allotropes" (Project #182849149).

O 41.2 Tue 18:00 P2/EG

Beyond Amorphous Carbon as an Embedding Material for Cluster Superlattice Membranes — •Stefan Schulte[1,2], Tobias Hartl[1], Alexei Preobrajenski[3], Jan Knudsen[3], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [3]MAX IV Laboratory, Lund University, Sweden

Cluster super lattice membranes constitute a novel 2D template material that has recently been described (T. Hartl et al., ACS Nano, 2020). So far, metal nano clusters on a graphene or hexagonal boron nitride support were embedded in an amorphous C matrix. This provides mechanical and thermal stability to the clusters, but a non-conductive embedding material, that allows for selective removal of the support structure is sought after. Here, embedding of cluster superlattices in B is presented and embedded clusters are characterized by STM and XPS. Embedding in B exhibit mechanical and thermal stability similar to amorphous C, e.g., Ir clusters on a graphene support embedded by a few monolayers of B remain in excellent order up to 750 K. This opens the pathway to electronic characterization of the nano clusters as well as removal of the support layer to expose stable clusters to ambient conditions. Further, preliminary results on CeO_2 embedding will be presented. CeO_2 embedded metal clusters are a promising material in few-atom catalysis processes.

O 41.3 Tue 18:00 P2/EG

H_2 Evolution from Methane Activated by Ta_8 Clusters on Pt(111) — •Matthias Knechtges, Tobias Hinke, Kevin Bertrang, Sebastian Kaiser, Nikita Levin, Martin Tschurl, and Ueli Heiz — TU Munich, School of Natural Sciences & Catalysis Research Center, Chair of Physical Chemistry

Methane as the main component of natural gas contains the highest energy density of all hydrocarbons but the activation poses great challenges, due to the high activation barrier of the C-H bonds.

Pathways to convert methane into valuable products at mild conditions are investigated in the UHV. Gas phase studies revealed that $Ta_8O_2^+$ catalytically converts methane to ethane and hydrogen at room temperature. The charge and oxygen density of the clusters appear to have great impact on their activity towards methane[1].

By employing a substrate manipulating the electronic and geometric structure of the clusters, the model system approaches to industrial heterogenous catalysis. Therefore, metallic Ta_8 clusters were deposited on different surfaces known for their electron drawing properties in analogy to the oxygen atoms in the $Ta_8O_2^+$. While no activity towards methane was observed Ta_8/SiO_2, hydrogen evolution was found after methane exposition on $Ta_8/Pt(111)$ in temperature programmed desorption(TPD) experiments.

Characterization by scanning tunnel microscopy showed randomly monodispersed flat arrangements and XPS to observe oxidation states.

[1] N.Levin et.al *J.Am.Chem.Soc.* **2020**, 142, 12, 5862-5869

O 41.4 Tue 18:00 P2/EG

Influence of Strong Metal-Support Interactions on the Photoactivity of Pt-loaded TiO_2(110) — •Lucia Mengel, Philip Petzoldt, 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

Pt-loaded TiO_2(110) is well-known for its capability of alcohol photoreforming. The hole-mediated photooxidation reaction yields hydrogen next to valuable organic compounds such as formaldehyde. The concept of encapsulation of clusters or nanoparticles by a metal oxide overlayer under reductive conditions is well established and has been extensively studied using a variety of techniques. Such encapsulations caused by strong metal-support interactions (SMSI) are a promising tool in photo-/electrocatalysis to improve catalyst selectivity and high-temperature stability. However, there is a lack of mechanistic understanding on the influence of an SMSI overlayer on the photocatalytic hydrogen evolution reaction.

In this poster, we discuss the influence of SMSI on the photoactivity of Pt-loaded TiO_2(110). As model reaction, methanol photoreforming is studied by catalytic measurements. We focus in particular on effects with relevance to the evolution of hydrogen, as TiO_x layers may impede the back reaction in full water splitting and thus have potential to replace currently predominant chromium oxide compounds.

O 42: Poster: Nanostructures at Surfaces

Time: Tuesday 18:00–20:00 Location: P2/EG

O 42.1 Tue 18:00 P2/EG

Nanostructuring of surfaces by slow highly charged ions — •Ayman El-Said[1], Rene Heller[2], and Stefan Facsko[2] — [1]Physics Department and Interdisciplinary Research Center for Advanced Materials, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Recently, considerable research efforts were devoted to the fabrication of extremely small nanostructures of significant potential in nanophotonics and nanoelectronics applications. Slow highly charged ions (HCI), as a promising nanotechnological tool, were successfully utilized for the creation of surface nanostructures in various solids [1]. Based on both the type of the material and ion beam parameters, nanostructures of different shapes (pits, caldera-like, hillocks) and sizes were obtained [2,3]. Here, we review the research progress on HCI-induced nanostructuring and the used theoretical approaches for understanding the creation mechanisms of the observed surface structures.

[1] A.S. El-Said, R.A. Wilhelm, R. Heller, M. Sorokin, S. Facsko, F. Aumayr, Phys Rev Lett 117, 126101 (2016).

[2] F. Aumayr, S. Facsko, A. S. El-Said, C. Trautmann, and M. Schleberger, J. Phys. Condens. Matter 23, 393001 (2011).

[3] S. Facsko, R. Heller, A.S. El-Said, W. Meissl, F. Aumayr, J. Phys. condensed matter 2, 224012 (2009).

O 42.2 Tue 18:00 P2/EG

Quantum simulator to emulate lower dimensional physics and chemistry — •E. Sierda, X. Huang, D. Badrtdinov, B. Kiraly, E. J. Knol, A.M.H. Krieg, N.M.M. Aarts, G. C. Groenenboom, M. I. Katsnelson, M. Rösner, D. Wegner, and A. A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

Designing materials with tailored physical and chemical properties requires a quantitative understanding of interacting quantum systems. In order to provide predictability, a promising route is to create bottom-up platforms, where the electronic properties of individual and interacting atoms can be emulated in a tunable manner. Here, we present a quantum simulator based on patterned Cs ions embedded in a 2DEG on the surface of semiconducting InSb(110). We use this platform to emulate the structure and orbital landscape of planar organic molecules. Using STM/STS and ab initio calculations, we show that an artificial atom can be derived from localized states of patterned Cs ions. The resultant potential can be used to couple artificial atoms, leading to bonding and anti-bonding states as well as to different orbital symmetries. Based on these artificial orbitals, we emulate molecular orbitals of known organic molecules, including antiaromatic molecules, based on various atomic structures. In a different limit where Cs atoms are much closer, this quantum simulator can also be used to probe the effect of e-e interactions. Our experimental data suggest that dense structures exhibit many-body effects which can be extended to complex quantum states based on arbitrary lattices.

O 42.3 Tue 18:00 P2/EG

Transition Metal Nanoparticles on Graphene: Influence of Temperature — •Kai Besocke, Mahboobeh Ravankhah, and Mathias Getzlaff — Institut für Angewandte Physik, Heinrich-Heine-Universität Düsseldorf

With its unique properties, such as high quality crystal structure, excellent electrical conductivity and high tensile strength, graphene is a promising substrate for fabricating nanocomposites.

In our research on supported transition metal nanoparticles we are investigating the influence of graphene as a substrate for the deposition of metallic nanoparticles and the influence of subsequent heating. In this contribution we present our results concerning the size distribution of $Fe_{0.5}Ni_{0.5}$-Nanoparticles on CVD-graphene surfaces.

The graphene surfaces are prepared on a cobalt thin film on a W(110) substrate. The particles under investigation are produced by means of Ar magnetron sputtering in a Haberland source and aggregation takes place in a He atmosphere. We analyze the behaviour of particles several nm in diameter at temperatures up to 500 °C.

Particle distributions are analyzed via STM and it will be discussed, whether the nanoparticles show different behaviour upon heating on graphene compared to other surfaces.

O 42.4 Tue 18:00 P2/EG

Activity of cerium oxide thin films prepared by atomic layer deposition using custom and commercial precursors — •Yuliia Kosto[1], Carlos Morales[1], Anjana Devi[2], Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Konrad-Zuse-Strasse 1, Cottbus 03046, Germany — [2]Inorganic Materials Chemistry, Ruhr University Bochum, Universitätsstraße 150, Bochum 44801, Germany

Atomic layer deposition (ALD) allows preparation of conformal coatings with possibility to control their thickness at the submonolayer level, making it a good tool for depositing active layers on 3D structures. Our group is working on cerium oxide-based materials for hydrogen detection, which is difficult at ambient conditions due to the low sensitivity and long response time of the sensors. The cerium oxide layers prepared by ALD contain a lot of defects and provide an opportunity to overcome these complications. Thickness and morphology of the oxide films play an important role in defining the Ce3+/Ce4+ ratio, as well as the interface with the used substrate. Here, we compare cerium oxide thin films deposited by ALD techniques on SiO2 and Al2O3 substrates. The results reveal that the interface to the substrate can considerably influence the reactivity of the cerium oxide toward hydrogen and oxygen. Preparation of the oxides using two different precursors (commercial Ce(thd)4 and custom Ce(dpdmg)3) has been demonstrated to affect the redox properties of the films, their reactivity, and the reversibility.

O 42.5 Tue 18:00 P2/EG

Local work function on Graphene Nanoribbons on Au(111) — •Daniel Rothhardt[1], Tilmann Klamroth[2], Amina Kimouche[1], and Regina Hoffmann-Vogel[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm, Germany — [2]Institute of Chemistry, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm, Germany

Graphene nanoribbons (GNRs) exhibit remarkable electronic properties due to the nature of the charge carriers and local confinements [1]. The local work function difference (LCDP) was investigated using an ultra-high-vacuum non-contact mode AFM and in addition to the topography, the local differences in the contact potential were recorded using the method of Kelvin Probe Force Microscopy. A charge transfer between the GNRs and the underlying gold substrate can be detected in the LCPD images which verifies the p-doping of the GNRS [2]. We observed a modification of the work function along the edges of the GNRs, which is due to the screening of the Au(111) of electrostatic fields from the GNR. Density functional theory (DFT) calculation supports the experimental findings.

[1] A.H. Castro, Neto et al , Rev. Mod. Phys. **81** , 109 (2009)

[2] D. Rothhardt et al , arXiv:2203.06945v1 , (2022)

O 42.6 Tue 18:00 P2/EG

Spin Switching in Self-Assembled Tetramers on Ag(111) — •Sven Johannsen[1], Sascha Ossinger[2], Sascha Schüddekopf[1], Jan Grunwald[3], Alexander Hermann[4], Troels Markussen[5], Heiko Wende[4], Felix Tuczek[3], Manuel Gruber[4], and Richard Berndt[1] — [1]Institute of Experimental and Applied Physics, CAU Kiel, Germany — [2]Department of Chemistry, University of Basel, Switzerland — [3]Institute of Inorganic Chemistry, CAU Kiel, Germany — [4]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [5]Synopsys Denmark, Fruebjergvej 3, 2100 Copenhagen, Denmark

Spin-crossover (SCO) molecules can be switched between a low spin (LS) state and a high spin (HS) state. Adsorption to a surface can lead to a drastic change of the SCO behaviour. We present a low-temperature scanning-tunneling-microscope investigation of the switching characteristics of metal-based SCO molecules organized in tetramers on a Ag(111) surface. Via the injection of current pulses two molecules per tetramer can be reversibly switched. In addition, these molecules may be switched remotely by applying the excitation to one of the other two molecules of the tetramers. The latter molecules themselves are immutable. We induced tens of thousands of switching events using different currents and voltages and observed that the switching yields that are 2 to 3 orders of magnitude larger compared to previous results. We show that the switching is likely linked to a spin transition and also report three-state switching that involves charging of a molecule.

O 42.7 Tue 18:00 P2/EG

Simulation of electronic transport in 2D networks — •Tim Güldenpfennig, Markus Gruschwitz, and Christoph Tegenkamp — Institut für Physik, TU Chemnitz, Reichenhainerstr. 70, 09126 Chemnitz

Interclation of atomic hydrogen into to the interface of buffer layer systems on SiC(0001) was shown to be powerful method to realize almost charge neutral quasi free monolayer graphene. This concept works also for intercalation of various metals (e.g. Pb, Sn, In) coming along with the formation of new 2D interface structures in proximity to graphene. However, defects within the buffer layer are often required for the intercalation of larger elements, thus the homogeneity of the intercalated areas depend strongly on the quality of the buffer layer and intercalation parameters. As a result, the quasi free monolayer graphene resembles a network structure rather than a homogeneous 2D phase.

In order to deduce the conductivity from our transport measurements done with a 4 point probe STM, we performed simulations. By means of COMSOL java api and the MPh library, the simulations were controlled via self-written python scripts. Next to the import of experimental data measured with high resolution SEM, own network structures were designed to study systematically the effect of anisotropy and inhomogeneities in 2D systems.

O 42.8 Tue 18:00 P2/EG

Preparation and STM study of clean Nb(111) surfaces — •Julia Goedecke[1], Maciej Bazarnik[2], and Roland Wiesendanger[1] — [1]Dept. of Physics, University of Hamburg, D-20355 Hamburg, Germany — [2]Institute of Physics, Poznan University of Technology, Piotrowo 3, 60-965 Poznan, Poland

Niobium with its highest transition temperature among all elemental superconductors has become a favorable substrate for realizing well-defined low-dimensional magnet-superconductor hybrid systems exhibiting novel types of exotic electronic states such as Majorana zero-energy modes. While a preparation procedure for obtaining atomically clean Nb(110) substrates has previously been reported, a suitable preparation method for clean Nb(111) surfaces is still lacking. Here, we report a recipe for cleaning Nb(111) surfaces based on an atomic hydrogen treatment followed by short flashes to elevated temperatures. The atomic surface structure of clean Nb(111) is investigated by high-resolution scanning tunneling microscopy (STM), revealing a surface reconstruction with a reduced atom density compared to the (111) plane of a bcc crystal.

O 42.9 Tue 18:00 P2/EG

Pulling single polar molecular wires by atomic force microscopy — •Christophe Nacci and Leonhard Grill — Institute of Chemistry, University of Graz, Graz, Austria

The frictional properties of individual nanostructures are strongly influenced by the low dimensionality and reduced size. Probing how they respond mechanically on different surfaces is essential to understand how the static and dynamic friction depend on the interplay between chemical composition and structural commensurability. Here, we report the vertical pulling of DAD molecular wires [1] off metal surfaces by non-contact atomic force microscopy (AFM), performed under ultrahigh vacuum and at low temperatures. The chemical structure of DAD polar wires is made of a regular alternation of donor (D) and acceptor (A) units. The mechanical response of single isolated molecular wires is probed by force spectroscopy. To further explore the role of structural commensurability between polymers and surface, the polar wires are also grown on ultrathin insulating NaCl films on metal surfaces.

[1] C. Nacci et al., Nature Comm. 6, 7397 (2015)

O 42.10 Tue 18:00 P2/EG

XRR Analysis of Al2O3 coated and mid-T baked niobium for future implementation in SIS-based SRF cavities — •Artem Zaidman[1,2], Getnet Kacha Deyu[2], Marc Wenskat[2], Vedran Vonk[1], Robert Zierold[3], Robert Blick[3,4], Wolfgang Hillert[2], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-SynchrDeutsches Elektronen-Synchrotron DESY, Germany — [2]Institute of Experimental Physics, Universität Hamburg, Germany — [3]Center for Hybrid Nanostructures (CHyN), Universität Hamburg, Germany — [4]Materials Science and Engineering, University of Wisconsin-Madison, United States

Bulk niobium is currently the most used material for RF surfaces. A new approach proposed by Gurevich [1] suggests the use of a superconductor-insulator-superconductor structure (SIS) to achieve higher accelerating fields and reduced surface resistance beyond the thermodynamic limits of Nb. As an intermediate step to pursue this model and in coordination with a similar procedure performed on a single-cell niobium cavity, a mechanically polished two-grain-Nb sample was coated with a 36 nm Al2O3 thin film via thermal atomic layer deposition (ALD) to create an insulating layer and baked for 3h at 300°C (mid-T bake) [2]. An XRR analysis of the sample was taken at each processing step to follow the changes in the niobium native oxide thickness and composition.

[1] A. Gurevich, Appl. Phys. Lett. 88, 012511 (2006) [2] S. Posen, et al., Phys. Rev. Applied 13, 014024 (2020)

O 42.11 Tue 18:00 P2/EG

Oxidation of α-Al$_2$O$_3$(0001)-supported Pt-Rh alloy nanoparticles — •Ming-Chao Kao, Simon Chung, Thomas F. Keller, Vedran Vonk, and Andreas Stierle — Deutsches Elektronen-Synchrotron DESY, Center for x-ray and Nanoscience CXNS, Hamburg 22607, Germany

Metal oxide supported platinum-rhodium bimetallic alloy nanoparticles are widely deployed in the field of heterogeneous catalysis, where they often undergo oxidation-reduction cycles. To better understand the oxidation process, we monitored the nanoparticles in-situ by Grazing Incidence X-ray Diffraction (GIXRD) as a function of different alloy compositions. By heteroepitaxial growth, α-Al$_2$O$_3$(0001) substrate supported Pt, Rh, and Pt-Rh alloy nanoparticles were grown via molecular beam epitaxy. The samples were characterized by SEM, AFM, XRR, and GIXRD. The aim of this study is to uncover the oxide formation on the NPs as a function of oxygen partial pressure and temperature. The oxidation experiment is performed with an in-situ oxidation chamber, which enables experiments to be carried out up to an oxygen pressure of 1000 mbar at 450°C. From the in-situ XRD experiments performed at constant temperature and increasing oxygen pressure, the following phenomena are deduced: particle sintering, selective oxidation, epitaxial strain, and the formation of Rh$_2$O$_3$ bulk oxide on (111)-oriented nanoparticles. Furthermore, composition-dependent changes together with selective oxidation and epitaxial strain were observed.

O 42.12 Tue 18:00 P2/EG

Structural and magnetic properties of epitaxial iron oxide nanoislands on SrTiO$_3$ — •Steffen Tober, Mai H. Hamed, Yifan Xu, Asmaa Qdemat, Connie Bednarski-Meinke, Ulrich Rücker, Oleg Petracic, Emmanuel Kentzinger, and Thomas Brückel — Jülich Centre for Neutron Science (JCNS) and Peter Grünberg Institut (PGI), JARA-FIT, Forschungszentrum Jülich

The chemical, electronic and magnetic properties of Fe$_x$O$_y$/oxide substrate heterostructures depend on substrate interactions and the flexible chemistry of the iron oxides, resulting in conductive or insulating, ferri- or antiferromagnetic phases. The reduced geometry of Fe$_{3-\delta}$O$_4$ nanoislands grown by reactive molecular beam epitaxy enables further tuning of electronic and magnetic properties for applications in catalysts and magnetoelectric devices [1]. We present the structural and magnetic characterisation of Fe$_{3-\delta}$O$_4$ nanoislands on (001) oriented SrTiO$_3$ with mixed SrO/TiO$_2$ and stepped TiO$_2$ surface terminations by reflection high-energy electron diffraction (RHEED), grazing incidence small angle X-ray scattering (GISAXS) and SQUID magnetometry [2,3]. Our findings indicate the growth of crystalline, evenly shaped, ferrimagnetic islands. These results form the basis for further experiments probing the local electronic and magnetic structure of the nanoislands.

[1] Y. Z. Chen et al., J. Appl. Phys. 103, 07D703 (2008), [2] G. E. Sterbinsky et al., J. Vac. Sci. Technol. B 25, 1389 (2007), [3] JCNS, JLSRF, 2, A61 (2016).

O 43: Poster: Plasmonics and Nanooptics I

Time: Tuesday 18:00–20:00 Location: P2/EG

O 43.1 Tue 18:00 P2/EG

Quantitative Modeling of Scattering-type Scanning Near-field Optical Microscope (s-SNOM) with the Finite Element Method Utilizing the Software JCMSuite — •Dinghe Dai, Dario Siebenkotten, Richard Ciesielski, and Bernd Kästner — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin

Scattering-type scanning near-field optical microscopy (s-SNOM), where local field enhancement is created with an oscillating nanotip, is widely applied in the nanoscale characterization of nanostructures, surface polaritons, and biomolecular systems. s-SNOM requires quantitative evaluation schemes with analytical models or simulation methods, among which the Finite Dipole Model [1] is a sophisticated model to calculate the near-field scattering for bulk materials. Nevertheless, it cannot model the full tip size or surface nanostructures. To solve this, a numerical model, based on the finite element method (FEM) software JCMSuite, is developed. The model describes the electromagnetic field over several orders of magnitude in physical size. At various infrared incident wavelengths (μm), the electromagnetic fields are simulated for different tip-sample gaps (nm) and demodulated at harmonics of the tapping frequency to eliminate background field effects. The agreement and deviation of amplitude and phase spectra between both models across multiple demodulation orders are discussed. The FEM by JCMSuite combined with field demodulation is a credible quantitative s-SNOM simulation method especially interesting for complex multilayer and nanooptical structures.
[1] Cvitkovic et al. Optics express 15(14) (2007): 8550-8565.

O 43.2 Tue 18:00 P2/EG

Switching nonlinear emission patterns of plasmonic nanostructures — •Valentin Dichtl, Kilian Wittman, Thorsten Schumacher, and Markus Lippitz — Experimental Physics III, University of Bayreuth, Germany

The nonlinear third-order material response of noble metals allows to shape the third-harmonic near field around a plasmonic nanostructure [1]. The corresponding spatial emission pattern of the third harmonic hot spots changes drastically when slightly tuning the fundamental wavelength over a linear resonance of the nanorod. This raises the question of whether similar behavior can be found for other nonlinear emission processes.

Here, we demonstrate by hyperspectral imaging that not only the third- but also the second-harmonic and especially the two- (or multi-) photon excited luminescence (TPPL) emission changes spatially, when tuning over the plasmon resonance. We discuss spatial and spectral differences between these processes.

The outlook is targeted towards selectively exciting single quantum emitters in the nearfield. As first step into this direction we present differences in the spatial change of luminescence of a dye film with respect to the underlying emission pattern.
[1] Wolf, D. *et al.* Shaping the nonlinear near field. *Nat. Commun.* 7:10361 (2016). doi: 10.1038/ncomms10361

O 43.3 Tue 18:00 P2/EG

Deep learning for the extraction of optical parameters of multilayer samples in scanning near-field optical microscopy — •Dario Siebenkotten, Lara Harren, Clemens Elster, and Bernd Kästner — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin

Scattering-type scanning near-field optical microscopy (s-SNOM) is a powerful method for optical material characterization at the nanoscale. However, owing to the complex interaction between tip and sample, extensive modelling is needed for the extraction of optical parameters, particularly for layered samples. The extraction of optical parameters typically requires fitting, which quickly becomes unstable [1] and can be very time intensive due to the complexity of the models. Deep Learning algorithms offer a fast alternative for the optical parameter extraction but have only been applied to bulk materials. Here, we show the extension of these approaches to systems consisting of one and two layers of polar crystals exhibiting surface phonon-polariton resonances on top of a substrate by training neural networks with model data. We present the trained neural networks and discuss the extraction accuracy for the cases of one and two layered samples. While this study is limited to polar crystals, the application to other systems, defined for example by free charge carriers or band transitions, is straight forward.
[1] McArdle et al. Phys. Rev. Research 2, 023272 (2020)

O 43.4 Tue 18:00 P2/EG

Nonlinear near-field optical microscopy (NNOM) for plasmonic skyrmions — •Florian Mangold, Bettina Frank, and Harald Giessen — 4th Physics Institute, Research Center SCoPE, and IQST, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

In recent years, plasmonic skyrmions have become a growing field of research. The state-of-the-art detection is done with PEEM (photoemission electron microscopy) or SNOM (scanning near-field optical microscopy) measurements.

An alternative to these methods is nonlinear near-field optical microscopy (NNOM) which uses an optical nonlinear process to image evanescent waves on the sub-wavelength-scale and enables real-time imaging of surface waves. By combining information from real and Fourier-space images, it is possible to calculate the phase and the amplitude of all electric field components.

The NNOM setup will be used to complement PEEM and SNOM measurements and gives us additional possibilities to investigate topological features in plasmonics such as quasicrystals, skyrmions and skyrmion bags.

O 43.5 Tue 18:00 P2/EG

Greyscale lithography with photoresist for plasmonic coupling — •Julian Alin, Michael Seidel, Thorsten Schumacher, and Markus Lippitz — Experimental Physics III, University of Bayreuth, Germany

Integrated plasmonic nanocircuits promise to play a major role for future applications of quantum optical technologies. Therefore stable, bright and narrow-band single-photon sources are required, such as self assembled epitaxially grown GaAs quantum dots [1]. Crucial for the coupling of such a quantum dot to a waveguide is, that for a high efficiency the waveguide has to be placed close to the quantum dot. However, the spatial proximity to the surrounding semiconductor material with a high refractive index strongly attenuates the surface plasmon propagation. In order to solve this problem we try to create a structure where the waveguide will be close to the quantum dot, but far away from the semiconductor material (a few hundred nanometers). To achieve this trough-like structure the idea is to apply a photoresist on a GaAs-sample, write a trough with a focussed gaussian laser beam and place a waveguide at this position. We discuss experiments on such structures with waveguides on glass substrates and first steps on GaAs wafers.

[1]Wu et al., Nano Lett. 2017, 17, 7, 4291-4296

O 43.6 Tue 18:00 P2/EG

Resistive heating of monocrystalline plasmonic resonators — •Jacob Syndikus, Luka Zurak, Jessica Meier, Bert Hecht, and Thorsten Feichtner — Nanooptics & Biophotonics Group, Experimental Physics 5, RCCM, JMU Würzburg, Am Hubland, D-97074 Würzburg, Germany

Plasmonic resonators can focus light down to sub-diffraction-limited near-field intensity volumes by collective oscillations of photons and electrons. Therefore, they are hot candidates for electro-optical devices with minimal footprint, bridging the gap between fiber communication and electronics or even being optical switches by themselves. To achieve this, the plasmonic properties have to be actively tuned, the faster the better.

Here we show experimentally the modulation of the wavelength dependent scattering intensity by a gold nanorod in the MHz range by resistive heating. Application of an AC voltage heats the gold material by several tens of Kelvin, changing the electron energy density and with it the dielectric constant ε_{Au}. The small volume and the electrical contacts ensure fast heat dissipation. We fabricate the structures from monocrystalline goldflakes by means of Ga- and He-ion beam milling and measure the changes in the resonance curves via white light laser illumination and modelocking detection. Numerical models show that GHz modulation is feasible to be realized which makes the technique interesting for applications.

O 43.7 Tue 18:00 P2/EG

Electrochemistry of the surface of electrically contacted plasmonic resonators — •Paul Mörk, Luka Zurak, Jessica Meier, Bert Hecht, and Thorsten Feichtner — Nano-Optics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Catalytic processes on gold surfaces are well known to enhance electrochemical processes. When the gold is showing geometric features on the nanometer scale, plasmonic resonances in the visible wavelength range can occur. This establishes addidional degrees of freedom (photon routing, heating, hot electron generation) to tailor an efficient material for photo-electrochemical processes interesting for energy applications like water splitting or CO_2 reduction.

Here we show the results of experiments with directly electrically connected plasmonic resonantors made via focused ion beam milling from monocrystalline gold flakes. Under ambient conditions without any further chemical added we observe a resonance shift by several ten of nanometers on a time scale of seconds when applying a electrical potential as high as 20 Volts to the gold surface. The effect reverses when the bias voltage is switched of on the time scale of hours. We present evidence that we observe the electrochemical oxidation and reduction of gold mediated by the omnipresent waterlayer covering every surface with nanometer thickness and deliver an outlook to the application within electrochemical cells.

O 43.8 Tue 18:00 P2/EG

Exciton lifetime of decoupled phthalocyanine molecules — •Amandeep Sagwal[1,2], Jiří Doležal[1], Rodrigo Cezar De Campos Ferreira[1], Petr Kahan[1], and Martin Švec[1,3] — [1]Institute of Physics, Czech Academy of Sciences; Praha, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University; Czech Republic — [3]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences; Czech Republic

A few layers of NaCl decoupling layer on metal are sufficient to prevent the nonradiative quenching of the excited state in phthalocyanine [1] and observe fluorescence in the far field from the molecule located in the junction of a scanning tunneling microscope (STM). First attempts to measure the lifetimes of exciton in the nanocavity suggested lifetimes of hundreds of picoseconds [2,3] but later studies pointed towards a transient charge state lifetime involved in the electroluminescence excitation process [4,5] and estimated the lifetime to be several orders of magnitude lower, due to the Purcell effect of the plasmonic nanocavity. Here, we use a pulsed supercontinuum laser to reveal the radiative decay of the excited state of the molecules with and without the presence of nanocavity.

[1]*F. Aguilar-Galindo et al. ACS Photonics 8, 3495 (2021) [2]*L. Zhang et al. Nat. Commun. 8, 580 (2017). [3]*J. Doležal et al. ACS Nano 15, 7694 (2021). [4] B. Yang et al. Nat. Photonics 14, 693 (2020). [5] K. Kaiser et al. arXiv:2211.01051 (2022).

O 44: Overview Talk Christian Ast

Time: Wednesday 9:30–10:15 Location: TRE Phy

Invited Talk O 44.1 Wed 9:30 TRE Phy

Spins on Surfaces: A Gateway to the Quantum World — •Christian R. Ast — MPI for Solid State Research, Stuttgart

Many exotic phenomena that are of current interest today rely on the quantum mechanical spin. With the focus on the atomic scale, placing spins on different surfaces has been a remarkably successful platform. Over the past decades, spins as they occur in atoms and molecules have been placed not only on insulating layers to decouple them from the environment and isolate their properties, but also on interacting normal and superconducting substrates. In this way, a plethora of different effects and concepts could be studied including, but not limited to the Kondo effect, Yu-Shiba-Rusinov states and by extension Majorana bound states, electron spin resonance as well as inelastic spin-flip spectroscopy. Here, I will present an overview of the field as well as recent developments in spins on surfaces at the atomic scale.

O 45: Focus Session: Scanning Probe Microscopy with Quartz Sensors I

Atomic Force Microscopy (AFM) was quickly adopted in science and engineering, but it took a while until the field of surface could benefit from it. 2023 marks the 25th anniversary of the introduction of the qPlus sensor. This stiff and self sensing force sensor made from quartz that often uses an etched metal tip as known from scanning tunneling microscopy (STM) replaced the silicon cantilever and allowed new types of experiments and new domains of precision. Scientists used it to resolve the structure of organic molecules with atomic resolution, to obtain subatomic spatial resolution, to image spin structures and spin lifetimes, to measure lateral forces, to detect tiny water molecules, to image oxides and other insulating surfaces with atomic resolution. Operation in ambient conditions, ultrahigh vacuum (UHV), low (4 K) and ultralow temperatures (10 mK) and in high magnetic fields as well as in an electrochemical cell was demonstrated.

Organizer: Franz Giessibl (U Regensburg)

Time: Wednesday 10:30–12:30 Location: CHE 89

O 45.1 Wed 10:30 CHE 89

The genesis of the qPlus sensor — •Franz Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, Universitätsstraße 31, 93053 Regensburg

In 1985, Gerd Binnig found exile from the STM frenzy at IBM Rüschlikon by a one year move to Stanford, the heart of silicon valley, and built the first atomic force microscope (AFM) together with Christoph Gerber and Calvin Quate [1]. Therefore, it is not surprising that the core of all AFMs, the cantilever, was soon micromachined from Si. Even the first successful imaging of Si 7x7 relied on piezoresistive Si cantilevers in the frequency modulation mode, albeit at an insanely large oscillation amplitude of 34 nm [2]. Benchmarking, widely used in management consulting, led to the conviction that quartz tuning forks with their utmost frequency stability would be a promising alternative. The phantastic frequency stability of the quartz forks used in Swatch watches and the realization that their stiffness allows sub-Angstrom oscillation amplitudes led to the invention of the qPlus sensor. Its stability, small amplitudes and low noise soon enabled subatomic resolution by AFM [3]. While qPlus sensors are standard in vacuum today, it is open if widespread application in ambient or liquid environments will become attractive, although atomic resolution has been demonstrated [4]. [1] G. Binnig, C.F. Quate, C. Gerber, Phys. Rev. Lett. 56, 930 (1986). [2] F.J. Giessibl, Science 267, 68 (1995). [3] F.J. Giessibl, S. Hembacher, H. Bielefeldt, J. Mannhart, Science 289, 422 (2000). [4] D.S. Wastl, A.J. Weymouth, F.J. Giessibl, Phys. Rev. B 87, 245415 (2013).

Topical Talk O 45.2 Wed 10:45 CHE 89

Single-molecule reactions performed and characterized using atomic force microscopy — •Leo Gross — IBM Research Europe - Zurich

Selective and reversible bond formation and dissociation can be controlled by tip-induced reduction-oxidation reactions on a surface. Molecular rearrangements leading to different constitutional isomers are selected by the polarity and magnitude of applied voltage pulses from the tip of a combined scanning tunneling microscope (STM) / atomic force microscope (AFM) [1].

Elusive molecules can be created and studied, such as cyclocarbons, i.e., molecular sp1 hybridized carbon allotropes [2] and molecules with high-spin ground states [3,4]. Moreover, insulating substrates allow probing charge states [5] and excited states [6].

References:
[1] F. Albrecht et al. Science. 377, 298-301 (2022).
[2] K. Kaiser et al. Science. 365, 1299-1301 (2019).
[3] N. Pavliček, et al. Nat. Nano. 12, 308-311 (2017).
[4] S. Mishra et al. ACS Nano. 16, 3264-3271 (2022).
[5] S. Fatayer et al. Science. 365, 142-145 (2019).
[6] S. Fatayer et al. Phys. Rev. Lett. 126, 176801 (2021).

O 45.3 Wed 11:15 CHE 89

On surface reaction of azaTrux molecules on Au (111) — •Outhmane Chahib[1], Jung-Ching Liu[1], Chao Li[1], Xunshan Liu[2], Uli Aschauer[2], Silvio Decurtins[2], Shi-Xia Liu[2], Ernst Meyer[1], and Rémy Pawlak[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland

One promising way to miniaturize electronic devices is to use "bottom-up" techniques, where functional organic molecules acting as elementary nanometer-sized "building blocks" are assembled or reacted on surfaces. Here we explore the on-surface reaction f 7,12-dibromo-5H-indeno[1,2-a]indolo-[3,2-c]carbazol-15(10H)-one molecules (AzaTrux) on the Au(111) surface into graphene nanostructures. Structural and electronic properties of nanostructures are characterized by scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with CO-terminated tips. Using force spectroscopy, we further probe the donor-acceptor character of these nanostructures.

O 45.4 Wed 11:30 CHE 89

A two dimensional array of radical molecules on Pb(111) — Jung-Ching Liu[1], Chao Li[1], H. Chen[2], Ping Zhou[3], Xunshan Liu[3], Ulrich Aschauer[3], Silvio Decurtins[3], Shi-Xia Liu[3], Wulf Wulfhekel[2], Ernst Meyer[1], and •Rémy Pawlak[1] — [1]University of Basel, Basel, Switzerland — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]University of Bern, Bern, Switzerland

The assembly of molecules to form a quantum dot array is of interest for quantum computing with the highest areal density. In this contribution, we show the supramolecular assembly of 4,5,9,10-tetrabromo-1,3,6,8-tetraazapyrene (TBTAP) molecules on superconducting Pb(111), self-organized in neighboring rows of radicals and neutral molecules [1]. By triggering a local field with a STM/AFM microscope at low temperature, we show that individual occupied molecules can be discharged efficiently, revealing Coulomb rings in spatial dI/dV maps. Charged molecules host spin 1/2, which is validated by dI/dV spectroscopy with μeV resolution through the observation of a pair of in-gap Yu-Shiba-Rusinov (YSR) states in the supraconducting gap. The unpaired electron cloud extends spatially over the entire molecule and interacts with neighbouring electrons, resulting in the formation of YSR bands along the entire molecular domain. [1] J.C. Liu et al. submitted.

O 45.5 Wed 11:45 CHE 89

Self-Assembly Study of 1,2,10,11,12,14-hexafluoropentacene on a Au(111) surface by HR-AFM — •Miguel Wiche[1], Maximilian Dreher[2], André Schirmeisen[1], Gregor Witte[2], and Daniel Ebeling[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Germany — [2]Fachbereich Physik, Philipps-Universität Marburg, Germany

The electronic properties of 2D organic materials highly depend on the orientation of the molecules inside the molecular thin film. For designing new materials with tailored functionality, it is important to understand the self-assembly processes of the individual molecular building blocks on surfaces. For example, the role of intermolecular halogen bonds for the molecular arrangement is not well understood. A powerful tool to investigate assembly processes in a step-by-step fashion is the bond imaging AFM method, which is based on operating qPlus sensors under UHV conditions at low temperatures with CO-functionalized tips. Here, the onset of the self-assembly process of individual partially fluorinated 1,2,10,11,12,14-hexafluoropentacene molecules on Au(111) is studied. Therefore, the molecules are first evaporated onto a cold surface (around 6K) where molecular diffusion is negligible. The formation of small clusters with closely packed molecules all facing in the same direction is induced by subsequent heating steps to temperatures up to 50K. At higher temperatures (80-300K) also larger islands form. After each heating step, the sample is cooled down to 5K for determining the precise bonding angles and length of the intermolecular $F\cdots H$ contacts via bond imaging AFM.

O 45.6 Wed 12:00 CHE 89

On-surface synthesis of PAHs by strain and the concerted motion of adatoms. — •Benjamin Mallada[1,2], Bruno de la Torre[1,2], Jesus I. Mendieta-Moreno[2], Adam Matej[1,2], Mikulas Matousek[3], Jiri Brabec[3], Libor Veis[3], Timothee Cadart[3], Martin Kotora[4], and Pavel Jelinek[1,2] — [1]Czech Advanced Technology and Research Institute (CATRIN), Olomouc, Czech Republic — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [3]J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic — [4]Department of Organic Chemistry, Charles University, Prague, Czech Republic

The kinetic control of the synthesis of polycyclic aromatic hydrocarbons (PAH) is one of the most desired features in organic synthesis. In this work, we report the synthesis and characterization by STM/nc-AFM of several PAHs from one single precursor in which two different kinetic-driven mechanisms control the possible products at high temperatures. In the first mechanism, we show that the surface-induced mechanical constraints on a strained helical reactant leads to the synthesis of planar objects with non-benzenoid rings. In the second mechanism, the chemical pathway is mediated by an unusual C-C bond cleavage of the helical reactant mediated by the concerted motion of individual gold adatoms. These observations, supported by DFT and state-of-the-art QM/MM calculations, render a scenario where the molecular internal stress and the adatoms' role enable routes to the kinetic control of selected chemical reactions.

O 45.7 Wed 12:15 CHE 89

Monitoring of molecular configurations in SPM-based molecular manipulation — Joshua Scheidt[1], Alexander Diener[1], Michael Maiworm[2], Klaus-Robert Müller[3], Rolf Findeisen[2], Kurt Driessens[4], F. Stefan Tautz[1], and •Christian Wagner[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Control and Cyber-Physical Systems Laboratory, Technische Universität Darmstadt, Germany — [3]Machine Learning Group, Technische Universität Berlin, Germany — [4]Data Science and Knowledge Engineering, Maastricht University, The Netherlands

Molecular manipulation with the SPM tip as an actuator allows creating a wide variety of molecular junction configurations. Unfortunately, the precise atomic locations in such a junction, which strongly impact its mechanical and electronic properties, cannot be observed directly. Here, we present and benchmark an approach that enables such a configuration monitoring. It overcomes the most important challenges: the need for accurate yet fast simulations, the disparity between scalar observation quantities like a force gradient and a high-dimensional unknown molecular configuration, the vast configuration space to be searched, and the need to operate on the few-minutes time scales of typical experiments. This is achieved by combining a finite state automaton to store and rapidly access the results of atomistic molecular simulations, and a particle filter to search for likely manipulation trajectories, given an input sequence of observations. We are able to assign systematic differences in generic features in force gradient data to well-defined atomic configurations for the first time.

O 46: Electron-Driven Processes at Surfaces and Interfaces

Time: Wednesday 10:30–12:15 Location: CHE 91

O 46.1 Wed 10:30 CHE 91

On the energy transfer mechanism in hyperthermal H atom scattering from surfaces — •Nils Hertl[1], Connor L. Box[1], and Reinhard J. Maurer[1,2] — [1]Department of Chemistry, University of Warwick, UK — [2]Department of Physics, University of Warwick, UK

Adsorption of atomic and molecular hydrogen on surfaces is the gateway to many important chemical processes in nature. Hence, it is important to understand their adsorption mechanism if we want to understand the relevant elementary processes of these adsorbates on surfaces.

In the recent years, a series of detailed theoretical and experimental investigations of energy transfer between H atoms and a variety of material surfaces have been performed. The investigated substrates range from noble gas surfaces with a detour to semiconductors to late fcc transition metal surfaces. Transition metal surfaces with adsorbates were investigated, too. For all studies, a UHV apparatus, specifically designed for H atom scattering, has been used. The complementary theory relies on molecular dynamics simulation, where electronic excitations are described within the framework of molecular dynamics with electronic friction. The friction coefficient is treated within the local density friction approximation (LDFA).

In this talk, I will briefly revisit those studies and on the basis of them, I will formulate a couple of general concepts relevant to atom scattering from surfaces. Furthermore, I will also present first efforts to apply methods which go beyond the framework of LDFA friction for hyperthermal H atom scattering.

O 46.2 Wed 10:45 CHE 91

Simulations of H atom scattering from p(2×2) O/Pt(111) surface with orbital-dependent friction — •Connor L. Box[1], Nils Hertl[1], and Reinhard J. Maurer[1,2] — [1]Department of Chemistry, University of Warwick, United Kingdom — [2]Department of Physics, University of Warwick, United Kingdom

The experimentally recorded nonadiabatic energy loss that occurs during H atom scattering from a range of clean metal surfaces is well reproduced by the molecular dynamics with electronic friction method using effective medium theory for the potential energy surface and the local-density friction approximation for the electronic friction. [1] However, it was recently reported that this method is not capable of reproducing the inelastic scattering of H atoms on the oxygen-covered Pt(111) surface. [2] We present inelastic scattering energy loss distributions for this system with an efficient ML representation of the orbital-dependent friction coefficients calculated using linear response theory based upon density functional theory. This approach additionally accounts for the anisotropy of the electronic friction tensor and the effect of the oxygen adatom on the surface electronic structure. [1] Dorenkamp et al, JCP, 2018 [2] Lecroart et al, JCP, 2021

O 46.3 Wed 11:00 CHE 91

Power discontinuity and shift of the energy onset of a molecular de-bromination reaction induced by hot-electron tunneling — Ana Barragan[1], Roberto Robles[1], Nicolas Lorente[1,3], and •Lucia Vitali[1,2,3] — [1]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), San Sebastián, Spain — [2]Ikerbasque Research Foundation for Science, Bilbao Spain — [3]Donostia International Physics Center (DIPC), San Sebastian

Understanding the mechanism of molecular dissociation under applied bias is a fundamental requirement to progress in (electro)- catalysis as well as in (opto)-electronics. The working conditions of a molecular-based device and the stability of chemical bonds can be addressed in metal*organic junctions by injecting electrons in tunneling conditions. Here, we have correlated the energy of debromination of an aryl group with its density of states in a self-assembled dimeric structure of 4'-bromo-4-mercaptobiphenyl adsorbed on an Au(111) surface. We have observed that the electron-energy range where the molecule is chemically stable can be extended, shifting the bias threshold for the rupture of the -C-Br bond continuously from about 2.4 to 4.4 V by changing the electron current. Correspondingly, the power needed for the dissociation drops sharply at 3.6 V, identifying different reaction regimes and the contribution of different molecular resonance states.

A.Barragan, R.Robles, N.Lorente, L.Vitali; Nanoscale 13, 15215 (2021)

O 46.4 Wed 11:15 CHE 91

Quantum transport on anisotropic surfaces revealed by MONA — •Manuel Seitz[1], Andreas Christ[1], Markus Leisegang[1], Jacek Waluk[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warsaw, Poland

The ability to detect how charge carriers propagate in well-defined bands is of great importance for the exploitation of novel materials, e.g., in the context of spintronics or topological insulators. We developed the molecular nanoprobe (MONA) technique [1] to investigate the details of quantum transport. It utilizes a single molecule to detect ballistic charge carriers injected by the tip of a scanning tunneling microscope (STM). In this study, we investigate charge carrier transport in the structurally anisotropic Cu(110) surface which exhibits a surface state at the Y-point of the surface Brillouin zone [2]. We performed directional-, distance-, and energy-dependent measurements that reveal an unexpectedly rich anisotropic behavior. The results can be explained by the combined influence of the band structure-dependent transport path and the molecular excitation.

[1] Leisegang, M. et. al., Nano Lett. 18, 2165 (2018).
[2] Jiang, J., et. al., Phys. Rev. B 89, 085404 (2014).

O 46.5 Wed 11:30 CHE 91

Understanding triplet-exciton transfer dynamics at the Si-tetracene interface — •Marvin Krenz — Universität Paderborn

Singlet-exciton fission in a tetracene overlayer and the subsequent triplet-exciton transfer into a silicon solar cell appears as promising approach to harvest high-energy photons [1]. However, the details of the exciton transfer and its dependence on the interface atomic structure are not understood. In the present contribution we employ ab initio non-adiabatic molecular dynamics to study the exciton transfer in atomistic detail. It is found that interface defects as well as thermal activation are instrumental for the exciton transfer from the organic overlayer into the Si bulk material.

[1] J.M. Luther, J.C. Johnson, Nature 571, 38 (2019)

O 46.6 Wed 11:45 CHE 91

Uni-directional translation of a novel adsorbate motor — •Grant J. Simpson[1], Mats Persson[2], and Leonhard Grill[1] — [1]University of Graz, Graz, Austria — [2]University of Liverpool, Liverpool, UK

Molecular motors are fascinating objects that can undergo uni-directional motion on the nanoscale. In order to independently perform meaningful work, they typically must switch between two potential energy surfaces to achieve directed motion. However, their rather complex structures often mean that their function on a surface is hindered. Here, we present a novel 'adsorbate motor' which performs strictly uni-directional translational upon excitation from the tip of a scanning tunneling microscope - in contrast to thermally induced motion of the same molecules that follows the principle of microscopic reversibility, resulting in random movement. The resulting 100% uni-directionality is then harnessed in order to perform meaningful work exemplified by the transport of single molecules across a metal surface.

O 46.7 Wed 12:00 CHE 91

Extreme magnetoresistance in high-mobility $Al_2O_3/SrTiO_3$ heterostructures — •Dennis Christensen — Technical University of Denmark, Department of Energy Conversion and Storage, 2800 Kgs Lyngby, Denmark

The heterostructure formed by depositing spinel γ-Al_2O_3 on perovskite $SrTiO_3$ exhibits a range of exciting properties including room temperature epitaxial growth [1,2], high electron mobility [3,4], a strain-tunable magnetic order [5] and a reordering of the t_{2g} bands due to the broken symmetry at the spinel/perovskite interface [6]. Here, I explore the magnetotransport properties of γ-$Al_2O_3/SrTiO_3$ and show that it exhibits a very large magnetoresistance exceeding 80,000% at 16 T and 2 K. When increasing the magnetic field, the field dependence of the magnetoresistance transitions from quadratic to linear with no saturation observed up to 16 T. I discuss the origin of this behaviour in relation to mechanisms known to produce large, unsaturated magnetoresistance.

[1] M. von Soosten, D. V. Christensen et al. Scientific Reports 9, 18005 (2019).

[2] Y. Z. Chen et al. Advanced Materials 26, 1462 (2014).

[3] Y. Z. Chen, N. Bovet, F. Trier, D. V. Christensen, et al. Nature Communications 4, 1371 (2013).

[4] D. V. Christensen, et al. Physical Review Applied 9, 054004 (2018).

[5] D. V. Christensen, et al. Nature Physics 15, 269 (2019).

[6] A. Chikina, D. V. Christensen et al. ACS Nano 15, 4347 (2021).

O 47: 2D Materials II: Growth, Structure and Substrate Interaction I

Time: Wednesday 10:30–13:00 Location: GER 37

O 47.1 Wed 10:30 GER 37

Two-Dimensional Non-van der Waals Materials from Data-Driven Research — Tom Barnowsky[1,2], Mahdi Ghorbani-Asl[1], Stefano Curtarolo[3], Arkady V. Krasheninnikov[1,4], and •Rico Friedrich[1,2,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]TU Dresden — [3]Duke University, Durham, USA — [4]Aalto University, Aalto, Finland

While two-dimensional (2D) materials are traditionally derived from bulk layered compounds bonded by weak van der Waals (vdW) forces, the recent surprising experimental realization of non-vdW 2D compounds obtained from non-layered crystals [1] foreshadows a new direction in 2D systems research.

Here, we present several dozens of candidates of this novel materials class derived from applying data-driven research methodologies in conjunction with autonomous *ab initio* calculations [2,3]. We find that the oxidation state of the surface cations of the 2D sheets is an enabling descriptor regarding the manufacturing of these systems as it determines their exfoliation energy: small oxidation states promote easy peel off [2]. When extending the set from oxides to sulfides and chlorides, the exfoliation energy becomes ultra low due to strong surface relaxations [3]. The candidates exhibit a wide range of appealing electronic, optical and magnetic properties making these systems an attractive platform for fundamental and applied nanoscience.

[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.*, submitted (2022).

O 47.2 Wed 10:45 GER 37

Phase Transitions of the BlueP-Au-network on Au(111) by Intercalation of Potassium — Philip Grimm, •Felix Otto, Maximilian Schaal, Florentine Friedrich, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

In 2014, a new elemental semiconductor was postulated: Blue Phosphorene (BlueP). This monolayer of P atoms offers a layer thickness-dependent band gap and high charge carrier mobility. However, the synthesis of a highly ordered and stable monolayer of BlueP is still a challenge and could only be achieved on gold substrates by constructing a Au-P network. This undesirable coupling, which leads to a change in electronic properties, could be mitigated by the intercalation of potassium. The goal is to synthesize a free-standing monolayer of BlueP. The effects of substrate temperature during K deposition and the order of deposition of phosphorus and potassium on Au(111) were investigated. Structural properties were characterized by LEED and RHEED, chemical properties by XPS, and electronic properties by photoelectron spectroscopy methods ((AR)UPS and PMM). In the end, a (2 × 2) superstructure is obtained. This superstructure exhibited the most promising electronic properties, which were very close to those of the free-standing BlueP. It is assumed that K and P together form the basis of the (2 × 2) superstructure, since the reactive bonds of potassium could be saturated and stabilized by phosphorus. At temperatures of 250 °C, the BlueP-Au network dissolves under the influence of potassium deposition and various intermediates are formed.

O 47.3 Wed 11:00 GER 37

Structural and chemical characterization of epitaxially grown $FeBr_2$ on Au(111) — •S. E. Hadjadj[1], C. Gonzalez-Orellana[2], J. Lawrence[3], D. Bikaljevic[4,5], M. Pena-Diaz[2], P. Gargiani[6], L. Aballe[6], J. Naumann[7], M. A. Nino[6], M. Foerster[6], S. Ruiz-Gomez[8], S. Thakur[1], I. Kumberg[1], J. Taylor[9], J. Hayes[1], J. Torres[1], C. Luo[9], F. Radu[9], D. G. de Oteyza[3], W. Kuch[1], J. I. Pascual[4], C. Rogero[2,3], and M. Ilyn[2] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Germany — [2]Centro de Fisica de Materiales, Donostia, Spain — [3]Donostia International Physics Center, Spain — [4]CIC nanoGUNE-BRTA, Donostia, Spain — [5]Institute of Physical Chemistry, University of Innsbruck, Austria — [6]ALBA Synchrotron Light Source, Spain — [7]Freie Universität Berlin, Dahlem Center for Complex Quantum Systems, Germany — [8]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [9]Helmholtz-Zentrum Berlin, Germany

We present structural, chemical and magnetic properties of the van–der–Waals material $FeBr_2$ on Au(111) with thicknesses from submonolayer to multilayer. We observe that the first layer on Au(111) shows a dominant superstructure. The chemical characterization by XPS and XAS shows that the material is growing in the same composition for different thicknesses. The magnetic characterization by XMCD reveals that the magnetic moment increases with increasing thickness.

O 47.4 Wed 11:15 GER 37

Formation of Europium transition metal surface compounds and its protection below hBN — •Alaa Mohammed Idris Bakhit[1,2], Khadiza Ali[3,4], Anna A. Makarova[4,5], Igor Piš[6], Federica Bondino[6], and Frederik Schiller[1,4] — [1]MPC, San Sebastián, Spain — [2]Universidad del País Vasco, San Sebastián, Spain — [3]Chalmers University of Technology, Göteborg, Sweden — [4]DIPC, San Sebastián, Spain — [5]FU Berlin, Germany — [6]IOM-CNR, Trieste, Italy

We present a comparative study of the electronic and structural properties of hBN on curved transition metal (TM) substrates, namely, Ni, Rh and Pt crystals and their modifications after Eu intercalation. hBN was grown by CVD processes. The growth quality depends strongly on the lattice mismatch and the overlayer-substrate interaction. The interface properties could be influenced by tuning the substrate material and its step density. That was shown by hBN growth on curved crystals that feature strong (Ni), medium (Rh) or weak (Pt) substrate interaction. The structural properties were investigated by Low-energy electron diffraction (LEED) and scanning tunnelling microscopy (STM). Stable facets are formed upon hBN growth on the substrates, which are changed after Eu intercalation. A formation of Eu-TM alloy is detected. The electronic structure was characterized by X-ray photoelectron spectroscopy (XPS) and angle-resolved photoemission measurements (ARPES). We studied the possible protection of Eu by the hBN layer. We observe that Eu protection was incomplete due to defects and hBN growth boundaries which resulted in Eu oxidation.

O 47.5 Wed 11:30 GER 37

Interaction of Au and Rh metals with h-BN on Rh(111) from theoretical calculations — •Krisztián Palotás — Wigner Research Center for Physics, Budapest, Hungary — ELKH-SZTE Reaction Kinetics and Surface Chemistry Research Group, Szeged, Hungary

Based on density functional theory calculations, the interaction of Au and Rh metal deposits with hexagonal boron nitride (h-BN) monolayer on a Rh(111) substrate in different model systems is studied. Significant differences in the metals' adsorption, growth and intercalation mechanisms are identified [1]. As an example, the formation of a 19-atoms Rh island in the pore of the nanomesh exhibits 3D growth, in contrast to a 2D island formation of Au [2]. We found that nitrogen vacancies and Rh show systematically lower energy barrier for atomic intercalation than boron vacancies and Au. Intercalation through the middle of a BN-divacancy provided the smallest energy barriers in our considered model systems. Our theoretical results provide a microscopic understanding of related experimental results [1].

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[1] G. Vári et al. submitted (2022). [2] A. P. Farkas et al. Appl. Catal. A Gen. 592, 117440 (2020).

O 47.6 Wed 11:45 GER 37

Local Electronic Structure of h-BN on Pt(110) — •Marco Thaler[1], Florian Mittendorfer[2], Erminald Bertel[1], and Laerte Patera[1] — [1]Institute of Physical Chemistry, University of Innsbruck, Austria — [2]Institute of Applied Physics and Center for Computational Materials Science, Vienna University of Technology, Austria

The growth of large-scale single-orientation hexagonal boron nitride (h-BN) monolayer has been recently achieved on the Pt(110) surface, exploiting the inversion of the normal substrate-adsorbate relation [1]. Here we performed Scanning Tunneling Spectroscopy to locally probe the electronic structure of h-BN and investigate the bonding configuration in detail. The moiré pattern arising from the mismatch with the substrate is observed to induce a modulation of the conduction band onset of h-BN and a shift of the Pt-related state, implying varying interaction energies. In agreement with density functional theory, the local density of states near the Fermi energy indicates a localized covalent bonding between h-BN and Pt, causing a (1xn)-missing row reconstruction of the Pt(110) surface. [1] D. Steiner, et al., ACS Nano, 13, 7083-7090 (2019).

O 47.7 Wed 12:00 GER 37

Chemical vapor deposition of high optical quality large area monolayer Janus transition metal dichalcogenides — •A. George[1], Z. Gan[1], I. Paradisanos[2], A. Estrada-Real[2], J. Picker[1], E. Najafidehaghani[1], F. Davies[3], C. Neumann[1], C. Robert[2], K. Watanabe[4], T. Taniguchi[4], X. Marie[2], J. Biskupek[5], M. Mundszinger[5], R. Leiter[5], U. Kaiser[5], A. Krasheninnikov[3], B. Urbaszek[2], and A. Turchanin[1] — [1]Friedrich Schiller University Jena, Jena, Germany — [2]Université de Toulouse, Toulouse, France — [3]Helmholtz-Centre Dresden Rossendorf, Dresden, Germany — [4]National Institute for Materials Science, Tsukuba, Japan — [5]University of Ulm, Ulm, Germany

Large scale chemical vapor deposition growth of Janus SeMoS monolayers is reported, with the asymmetric top (Se) and bottom (S) chalcogen atomic planes with respect to the central transition metal (Mo) atoms. The formation of these 2D semiconductor monolayers takes place upon the thermodynamically driven exchange of the bottom Se atoms of the initially grown MoSe$_2$ single crystals on gold foils with S atoms. The growth process is characterized by complementary experimental techniques including Raman and X-ray photoelectron spectroscopy, transmission electron microscopy, and the growth mechanisms are rationalized by first-principles calculations. The remarkably high optical quality of the synthesized Janus monolayers is demonstrated by optical and magneto-optical measurements which reveal the strong exciton-phonon coupling and enable to obtain an exciton g-factor of -3.3. (Adv. Mater. 34, 2022, 2205226)

O 47.8 Wed 12:15 GER 37

Preparation and characterization of carborane based nanomembranes — •Martha Frey[1], Julian Picker[1], Jakub Višňák[2], Christof Neumann[1], Tomáš Baše[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]The Czech Academy of Sciences, Institute of Inorganic Chemistry, 250 68 Husinec-Rez, c.p. 1001, Czech Republic

Carboranes are electron-delocalized molecular clusters containing boron, carbon, and hydrogen. Because of their high chemical and thermal stability as well as their structural variability, they are interesting for a wide range of applications including nanoscale engineering, catalysis, and boron neutron capture therapy. Here, we present the fabrication of a novel boron-based two-dimensional (2D) material *via* electron irradiation induced cross-linking of carborane self-assembled monolayers (SAMs) on silver substrates. Using the double-cage molecule 1,2-dicarba-*closo*-dodecaborane-9,12-dithiol, the fabrication of a mechanically stable and continuous ∼1 nm thin membrane was achieved. The self-assembly, cross-linking and transfer of the resulting nanomembranes onto grids have been characterized with different complementary surface-sensitive techniques including X-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED), ultraviolet photoelectron spectroscopy (UPS) and scanning electron microscopy (SEM).

O 47.9 Wed 12:30 GER 37

A Metastable Pentagonal 2D Material Synthesized by Symmetry-Driven Epitaxy — •Lina Liu[1,2] and Yong Chen[1,2] — [1]Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana, 47907, USA — [2]Institute of Physics and Astronomy and Villum Centers for Dirac Materials and for Hybrid Quantum Materials and Devices, Aarhus University, 8000 Aarhus-C, Denmark

Most two-dimensional (2D) materials experimentally studied so far have hexagons as their building blocks. Only a few exceptions, such as PdSe2, are lower in energy in pentagonal phases and exhibit pentagons as the building blocks. Such pentagonal 2D materials demonstrate unprecedented properties and unique applications originated from low-symmetry lattice geometries. While theory has predicted a large number of pentagonal 2D materials, many of them are metastable and their experimental realization is difficult. Here, we report the first synthesis of a metastable pentagonal 2D material, the pentagonal PdTe2 monolayer, by symmetry-driven epitaxy. Scanning tunneling microscopy is used to characterize the monolayer pentagonal PdTe2, which demonstrates well-ordered low-symmetry atomic arrangements. Theoretical calculations, along with angle-resolved photoemission spectroscopy, reveal the band structures of monolayer pentagonal PdTe2. In contrast to the narrow bandgap of monolayer hexagonal PdTe2, monolayer pentagonal PdTe2 is a semiconductor with a much bigger indirect bandgap of 1.08 eV. Our work opens an avenue for the synthesis of new, pentagon-based 2D materials and gives great opportunities to explore their applications such as multifunctional electronics.

O 47.10 Wed 12:45 GER 37

The transformation of 2D honeycombs into dodecagonal quasicrystals — •Stefan Förster, Loi Vinh Tran, Martin Haller, Sebastian Schenk, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Oxide quasicrystals are 2D materials with an aperiodic dodecagonal symmetry [1]. Starting from a binary oxide Ti$_2$O$_3$ honeycomb structure on Pt(111), the Ti$_n$O$_n$ ring structure with n=6 is transformed into a network of rings with ring sizes of n= 4, 5, 7 and 10 in the presence of Ba atoms. In these networks, n=7 rings host one Ba atom and n=10 rings host two [23].

In this contribution, the basic mechanisms for the network transformation are discussed. Stone-Wales transformations are the key mechanism to realize n=4...7 rings. In addition, by incorporating an additional oxygen atom, two neighboring n=6 rings convert into a n=10 ring [3]. The amount of Ba controls this conversion process and leads to a sequence of long-range ordered structures including a well-defined quasicrystal.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, Nature **502**, 215 (2013)
[2] E. Cockayne et. al, Phys. Rev. B **93**, 020101(R) (2016)
[3] S. Schenk, O. Krahn, E. Cockayne, H. L. Meyerheim, M. De-Boissieu, S. Förster, and W. Widdra, Nat. Commun, accepted (2022)

O 48: Focus Session: Semiconductor Surface Chemistry – from Reaction Mechanisms to Well-Ordered Interfaces I

The interest in the properties of semiconductor surfaces and chemical reactions on these surfaces is driven by a large range of current and future applications. They are spanning from conventional microelectronics over molecular electronics, atomic scale and quantum devices to photo(-electro)-chemical processes for large-scale synthesis of chemicals such as hydrogen and ammonia. In this focus session, the wide variety of topics in semiconductor surface chemistry is illustrated in the same way as the common aspects of the field are emphasized. In particular, the question how to control the reactivity on semiconductor surfaces, which is typically governed by the high localization of charge at the surface dangling bonds, will be addressed for the different systems. A larger part of the session will be dedicated to the reaction of organic molecules on semiconductor surfaces and how the control of these reactions can lead to the synthesis of ordered organic architectures with well-controlled properties on semiconductor surfaces.

Organizer: Michael Dürr (U Giessen)

Time: Wednesday 10:30–12:15 Location: GER 38

Topical Talk O 48.1 Wed 10:30 GER 38

Surface functionalization of semiconductors: Introducing spectroscopic labels, monolayer control for ultra-shallow doping, and providing surface passivation for atomically-precise processes — •Andrew Teplyakov — 112 Lammot DuPont Laboratory, Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716, USA

Over the last several decades, chemistry for surface functionalization of semiconductors went through a number of directional changes that were largely dictated by the technology development. Some of the recent work in our group has been targeting modification of both flat surfaces and the surfaces of nanoparticular semiconductor materials to introduce spectroscopic labels, provide monolayer control for ultra-shallow doping, and also to control the passivation of surfaces for atomically-precise processes. This presentation will start with applying the basic principles of surface chemical design to silicon surfaces. Specifically, I will cover the solution reactions of boron- and nitrogen-containing compounds with hydrogen- and chlorine-terminated silicon surfaces. Parallels and major differences between the chemistry of (100) and (111) crystal faces of silicon will be examined. The reactions of the same surfaces with metalorganic precursor molecules will be presented to evaluate the role of minority sites (defects) in atomically-precise processing. Finally, the parallels between surface chemical modification of flat silicon surfaces and metal oxide nanomaterials will be examined and the challenges in connecting physical and chemical properties of these materials will be evaluated.

O 48.2 Wed 11:00 GER 38

Theoretical studies on surface stabilities of $FeCuO_2$ and $CuBi_2O_4$ — •Julian Bessner, Stefanie Bogenrieder, Björn Kirchhoff, and Timo Jacob — Ulm University, Institute of Electrochemistry, D-89081 Ulm

Ammonia is the most important component in fertilizers, as 80% of the worldwide production goes into fertilizers.[1] Currently, the energetically expensive Haber-Bosch process is used to break the triple bond of N_2. In the last years, the photoelectrochemical (PEC) reduction of nitrogen has gained attention, providing a more affordable and sustainable ammonia production. To this end, $CuFeO_2$ and $CuBi_2O_4$ are investigated as materials for photocathodes as promising alternatives for the conversion of solar energy into chemical fuels.[2, 3] So far, most theoretical and experimental studies on these materials had focused on bulk properties. Here, we perform Density Functional Theory calculations (DFT+U) to analyze their electronic properties, thermodynamic stability of different surfaces and adsorption energy trends for the nitrogen reduction reaction (NRR) intermediates. Additionally, the influence of an aqueous surrounding on the stability of the surfaces and reaction intermediates thereon will be investigated using the hybrid QMMM simulation approach (SAFIRES) implemented in ASE and GPAW, which to this end will be extended to be compatible with periodic surface models.

[1] Smil, V. Nature 400, 1999, 415.
[2] Jiang, C.-M. et al. Chem. Mater., 31, 7, 2019, 2524-2534
[3] Ferri, M. et al. ACS Catalysis 11 (4), 2021, 1897-1910.

Topical Talk O 48.3 Wed 11:15 GER 38

Growth of organic monolayers on Si(111) — •Martin Franz — Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany

The ever-growing number of semiconductor based applications leads to an increasing demand for a modification or functionalization of surfaces with organic molecules. However, while the formation of self-assembled monolayers of organic molecules is well established on metal surfaces, the high density of dangling bonds present on most clean semiconductor surfaces typically reduces the mobility of molecules preventing an ordered growth. A route to overcome this constraint is the modification of the surface, allowing to precisely adjust the substrate-molecule interaction enabling a controlled growth.

In this talk, examples of organic films on modified Si(111) surfaces are given, which were investigated using scanning tunneling microscopy as well as tunneling and photoelectron spectroscopy. A prominent example in this regard is the boron-modified Si(111)$\sqrt{3} \times \sqrt{3}$R30°-B surface. Here, results for N-heterocyclic carbenes, which form highly ordered monolayers with promising properties [1], and for cobalt phthalocyanine [2-3] are discussed. Further examples given include the influence of surface defects on the molecular adsorption process and the use of indium-modified Si(111) as substrate [4].

[1] M. Franz et al., Nat. Chem. **13**, 828 (2021).
[2] S. Lindner et al., Phys. Rev. B **100**, 245301 (2019).
[3] H. Aldahhak et al., Phys. Rev. B **103**, 035303 (2021).
[4] M. Kubicki et al., Appl. Phys. Lett. **119**, 133105 (2021).

O 48.4 Wed 11:45 GER 38

Organic molecular architectures synthesized by means of solution-based click chemistry on functionalized silicon surfaces — •Timo Glaser[1], Jannick Alexander Peters[1], Christian Länger[1], Dominik Scharf[2], Jannick Meinecke[2], Ulrich Koert[2], and Michael Dürr[1] — [1]Institut für Angewandte Physik und Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Fachbereich Chemie, Philipps-Universität Marburg, Germany

The application of organic click chemistry to selectively functionalized silicon surfaces may open the route to synthesizing new organic molecular architectures on silicon. However, this scheme seems to be an experimental contradiction since click reactions are performed in the presence of a catalyst dissolved in a solvent whereas the highly reactive Si(001) surface is prepared and stored under UHV conditions. Here we show how to combine surface functionalization performed under UHV conditions with solution-based alkyne-azide click reactions. The UHV-based functionalization of Si(001) was realized via chemoselective adsorption of ethinyl cyclopropyl cyclooctyne (ECCO) from the gas phase. The samples were then directly transferred from UHV into the reaction solution where alternating layers of bisazide and bisalkine were coupled subsequently step by step without exposure to ambient conditions. Each reaction step was monitored by means of XPS in UHV and the selectivity of the reaction schemes in use was demonstrated. Using optimized copper(I) catalysts, reaction yields of up to 75 % were obtained.

O 48.5 Wed 12:00 GER 38

Towards Ab Initio Design of Internal Interfaces - The Adsorp-

tion of Cyclooctyne on Semiconductor Surfaces — •Hendrik Weiske and Ralf Tonner-Zech — Universität Leipzig, Germany

Modern Society is massively influenced by technological progress, specifically the development of the electronics industry. The controlled functionalization of semiconductor interfaces with organic molecules offers new possibilities to advance the application range of classical semiconductors. The chemoselective attachment of multifunctional organic molecules is the first step in forming well-defined organic/semiconductor interfaces.
Previously, we investigated the functionalization of Si(001) surfaces extensively [1,2]. This research focussed on bifunctional cyclooctyne, which attaches to Si(001) via its strained triple bond. This work is extended here to various semiconducting substrates, such as Ge(001), to predict new and promising interfaces. The reactivity and fundamental bonding interactions are studied using various computational methods, such as the pEDA, AIMD, and NEB.
We acknowledge funding from the DFG via SFB1083.

References

[1] F. Pieck, R. Tonner-Zech, *Molecules* **2021**, *26*, 6653
[2] L. Pecher, S. Schmidt, R. Tonner, *J. Phys. Chem. C*, **2017**, *121*, 26840-26850

O 49: Plasmonics and Nanooptics I: Fabrication and Application

Time: Wednesday 10:30–12:45 Location: WIL A317

O 49.1 Wed 10:30 WIL A317

Towards dynamic holograms with electrically switchable polymer metasurfaces: materials apsects — •Dominik Ludescher, Julian Karst, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Holography is considered as an innovative technology that is predicted to have a significant impact on numerous fields of application such as virtual, mixed, augmented reality, medical technology, and future displays. Overlaying digital information with the real world is the general concept of augmented reality. Yet, for concepts such as 3D holographic video conferencing or surgery planning, high-resolution and high-performance dynamic holograms are inevitable. To achieve this goal, nanophotonic plasmonic approaches are considered as a very promising platform. Here, we introduce active plasmonic metasurfaces for dynamic holography based on electrically switchable metallic polymer nanoantennas. The used polymer material incorporates a metal-to-insulator phase transition in the infrared spectral range which is driven by CMOS compatible voltages of only +/-1 V. In combination with possible pixel sizes below 1 micron, this makes the polymer metasurface ideally suited for holographic display applications. Additionally, using variable angle spectroscopic ellipsometry, we investigate the optical properties of such metallic polymers. In particular, we analyze their complex dielectric function and the associated zero epsilon region around the plasma wavelength. This will lay the foundation to shift the plasmonic metasurface operation to the visible spectral range.

O 49.2 Wed 10:45 WIL A317

Sampling polar THz nearfields using nonpolar Stark-effect — •Moritz B. Heindl[1], Nicholas Kirkwood[2], Tobias Lauster[3], Markus Retsch[3], Paul Mulvaney[2], and Georg Herink[1] — [1]Experimental Physics VIII, University of Bayreuth, Germany — [2]ARC Centre of Excellence in Exciton Science, School of Chemistry, University of Melbourne, Australia — [3]Physical Chemistry I, University of Bayreuth, Germany

Quantum-Probe Field Microscopy (QFIM) enables the imaging of ultrafast THz nearfield waveforms with a conventional fluorescence microscope at optical resolution [1]. Although the underlying quantum-confined Stark-effect scales quadratically in typical configurations, we are able to resolve the full polarity of the THz nearfields utilizing alternative approaches. Specifically, we employ a carrier-envelope phase shift of the driving THz waveform or external biasing of the THz nearfield, as we discuss in this contribution.

[1] Heindl, M. B. et al. Light Sci. Appl. 11, 5 (2022)

O 49.3 Wed 11:00 WIL A317

Double resonant, monocrystalline plasmonic gratings evolutionary optimized for enhanced SERS sensing — •Thorsten Feichtner[1], Katja Höflich[2], Enno Schatz[1], Amro Swedan[3], Paul Mörk[1], and Muhammad Bashouti[3,4] — [1]Nanooptics & Biophotonics Group, Experimental Physics 5, RCCM, JMU Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Photonic Quantum Technologies, FBH gGmbH Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, D-12489 Berlin, Germany — [3]IKI for Nanoscale Science & Technology, BGU of the Negev, Beer-Sheva 8410501, Israel — [4]Department of Solar Energy and Environmental Physics, SIDEER, J. Blaustein Institutes for Desert Research, BGU of the Negev, Midreshet Ben-Gurion, 8499000, Israel

Surface enhanced Raman spectroscopy (SERS) is an extremely sensitive non-linear method to detect vibrational energy levels of molecules using visible light. However, most SERS substrates available today are quite inhomogeneous.

Here we provide experimental evidence of an efficient and homogeneous SERS substrate consisting of numerically evolutionary optimized two-dimensional gratings made from straight monocrystalline metal wires. The combination of grating resonance and plasmonic gap resonance allows to enhance both excitation of the molecules and emission of the Raman signal, which have to be treated separately to unlock the full potential of SERS. Many experiments comparing gratings, materials and analytes will be presented to illustrate the underlying physical mechanisms and the huge potential for applications.

O 49.4 Wed 11:15 WIL A317

Topological insulating phase in non-Hermitian plasmonic waveguide arrays — •Helene Wetter[1], Stefan Linden[1], and Julian Schmitt[2] — [1]Physikalisches Institut, Universität Bonn, Kreuzbergweg 24, 53115-Bonn, Germany — [2]Institut für Angewandte Physik, Universität Bonn, Wegelerstr. 8, 53115-Bonn, Germany

Arrays of evanescently coupled plasmonic waveguides are a powerful platform to investigate topological properties of one-dimensional lattices. The underlying principle is the mathematical equivalence between the single-particle tight-binding Schrödinger equation and the coupled mode equation. By tailoring the loss distribution, we utilize non-Hermiticity as a new approach to induce topological phases in otherwise trivial systems. We employ dielectric loaded surface plasmon polariton waveguides fabricated on a thin gold film. Additional losses are introduced to specific waveguides by deposition of a thin layer of chromium below the respective waveguides. Considering a unit cell of four waveguides, a topologically nontrivial lattice can be created by adding an equal amount of losses to the two central waveguides of the unit cell. In contrast, losses on either the first or the last two waveguides of a unit cell correspond to a trivial lattice. Using leakage radiation microscopy, we observe localized states at the edge of the nontrivial lattice (edge mode) as well as at the interface between the nontrivial and the trivial lattice (interface mode). Conversely, the trivial lattice does not provide a localized edge mode. Thus, the topological properties can solely be controlled by the design of the unit cell.

O 49.5 Wed 11:30 WIL A317

Plasmonics of Silica Encapsulated Au@Ag Nanoparticles — •Johannes Schultz[1], Felizitas Kirner[2], Pavel Potapov[1], Bernd Büchner[1,3], Axel Lubk[1,3], and Elena Sturm[2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e. V., Helmholtzstraße 20, 01069 Dresden — [2]Department of Chemistry, University of Konstanz, Universitätsstraße 10, 78457 Konstanz — [3]Institute of Solid State and Materials Physics, Haeckelstraße 3, 01069 Dresden

Localized Surface Plasmons (LSPs) are collective charge oscillations arising at interfaces between media of opposite sign of the corresponding dielectric functions. Here, spatial confinement of the LSPs, e.g. in nanoparticles (NPs), may lead to resonant amplification of the corresponding electromagnetic (e.m.) fields. This effect is exploited in several application, e.g., surface enhanced Raman spectroscopy or plasmonic solar cells. Depending on the application, this requires specific control of the spectral positions of the LSPs. Since the latter depend on both, the dielectric function of the NP and the surrounding, tuning of the LSPs can be realized by varying the dielectric environment of the NP. Here, a novel synthesis method was used to encapsulate silver nanocubes with silica layers of uniform and adjustable thickness in the range between 8 and 22 nm to tune the dielectric environment and hence the excitation energies of the LSPs with high precision over a broad spectral range between 2.55 and 3.25 eV. Furthermore, resonant coupling between Mie-type resonances at the silica-vacuum interface and the LSPs was found which leads to an e.m. field enhancement in the range of 100 %.

O 49.6 Wed 11:45 WIL A317

Strain-driven thermal and optical instability in Ag/a-Si hyperbolic metamaterials — •Lea Forster[1,2], Jose L. Ocana-Pujol[1], Ralph Spolenak[1], and Henning Galinski[1] — [1]Laboratory of Nanometallurgy, ETH Zurich, Switzerland — [2]Laboratory for Multifunctional Ferroic Materials, ETH Zurich, Switzerland

In a hyperbolic metamaterial system of silver/amorphous-silicon multilayers we investigated the thermal instability which arises upon heating. Our analysis demonstrates that this instability is governed by the minimization of interfacial energy and anisotropic elastic strain energy caused by the mismatch of thermal expansion coefficients. Interestingly, the stacking order of the multilayer influences which of these two energy contributions dominates. We observed this behavior by a combination of FIB-SEM tomography, finite element simulations, and optical spectroscopy. Our results show that the thermal instability initiates at 300 °C, while the hyperbolic dispersion despite increased structural disorder persists up to 500 °C. These findings can lead to a better understanding of thermal instabilities in multilayers and may assist in the design of hyperbolic metamaterials for high-temperature applications.

O 49.7 Wed 12:00 WIL A317

Optical grating couplers for the excitation of Bloch surface waves — •Sebastian Henn, Marius Grundmann, and Chris Sturm — Universität Leipzig, Faculty of Physics and Earth Sciences, Felix Bloch Institute for Solid State Physics, Linnéstr. 5, 04103 Leipzig, Germany

In this contribution we demonstrate experimentally the control of the propagation of Bloch Surface Waves (BSW) in the transparent spectral range. BSW exist along the interface of a distributed Bragg reflector (DBR) with a thin top layer of a specified thickness to the ambient. Using shallow optical diffraction gratings with a sub-micron lattice constant, incident light is coupled into and out of the Bloch modes, which propagate along the surface between the gratings. The low-loss nature of evanescent BSW leads to long-range lateral propagation, on the order of micrometers, making this an interesting candidate for on-chip devices, for example by coupling to excitons, i.e. exciton-polariton applications. We give an overview of the fabrication processes as well as the results regarding the optical excitation of BSW by means of imaging ellipsometry, which is supported by rigorous coupled-wave analysis modelling.

O 49.8 Wed 12:15 WIL A317

Reconfigurable and polarization-dependent perfect absorber for large-area emissivity control based on the plasmonic phase-change material In_3SbTe_2 — •Lukas Conrads[1], Natalie Honné[1], Andreas Ulm[2], Andreas Hessler[1], Matthias Wuttig[1], Robert Schmitt[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Fraunhofer IPT

Metasurfaces with perfect infrared absorption promise integrated filters and compact, tailorable detector elements for thermal radiation. Phase-change materials (PCMs) are prime candidates for active, nonvolatile absorption tuning [1]. In this work, we show flexible encoding of different absorption/emission properties within a metasurface. We employ the plasmonic PCM In_3SbTe_2 (IST) [2] to obtain control over the emissivity by patterning an adaptable perfect absorber metasurface. Using a commercial direct laser writing setup, we locally switch the IST from an amorphous dielectric into a crystalline metallic state and write nanoscale stripe gratings of cm-size above a reflecting mirror. We demonstrate modification of already written patterns by changing the laser power and thus the IST stripe width to encode different polarization-sensitive patterns with nearly perfect absorption into the same metasurface. Finally, we measure an apparent local temperature pattern due to our large-area emissivity shaping metasurface with a conventional thermal camera [3]. Our results pave the way towards low-cost, large-area and adaptable patterning of metasurfaces.

[1] Wuttig et al. *Nat. Photon.* **11**, 465 (2017) [2] Heßler et al. *Nat. Commu.* **12**, 924 (2021) [3] Conrads et al. *Adv. Opt. Mat.* submitted

O 49.9 Wed 12:30 WIL A317

Sensing at the ultimate volume limit: Refractive index sensing in attoliter volumes using Mie voids — •Serkan Arslan[1], Huong Tran[1], Julian Karst[1], Lida Shamsafar[1], Thomas Weiss[2], Harald Giessen[1], and Mario Hentschel[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart, Germany — [2]Institute of Physics, University of Graz, and NAWI Graz, 8010 Graz, Austria

Traditional nanophotonic sensing schemes utilize dielectric or metallic nanoparticles, which confine far-field radiation in dispersive and lossy media. Apart from ill-defined sensing volumes and moderate sensitivities, these structures suffer from the generally limited access to the modal field, which is key for sensing performance. Recently, a novel strategy for dielectric nanophotonics has been demonstrated, namely, the resonant confinement of light in air. Voids created in high-index dielectric host materials support localized resonant modes with exceptional properties. In particular, due to the confinement in air, these structures benefit from the full access to the modal field inside the void. We utilize these so-called Mie voids for refractive index sensing on the single void level with unprecedented small sensing volumes in the range of 100 attoliter and sensitivities on the order of 500 nm per refractive index unit. Strikingly, the sensitivity as well as the scattering cross sections of the voids are large enough to even identify different analytes with bare eye in an optical microscope. The combination of our Mie void sensor platform with appropriate surface functionalization will even enable specificity to biological or other analytes of interest.

O 50: Spins on Surfaces at the Atomic Scale IV

Time: Wednesday 10:30–11:30 Location: REC C 213

O 50.1 Wed 10:30 REC C 213

Growth and magnetism of ultrathin Fe films on Ta(110) — •Reiner Brüning, Roberto Lo Conte, Kirsten von Bergmann, and Roland Wiesendanger — Institut für Nanostruktur- und Festkörperphysik, Universität Hamburg

The field of hybrid systems, where magnetism and superconductivity are interacting with each other, is a field which is attracting more and more attention in recent years. Spin-polarized scanning tunneling microscopy (SP-STM) is an ideal tool to study the magnetic as well as the superconducting properties and investigate the interplay between each other.

Here, we investigate ultrathin Fe films on the anisotropic (110) surface of the elemental superconductor Ta by SP-STM. For the pseudomorphic Fe monolayer, theory has predicted [1] interesting magnetic ground states depending on the interlayer distance [1], e. g. a magnetic spin spiral with a period of 6 nm.

We observe pseudomorphic growth for sub-monolayer coverage, however, for higher coverage we find several different structures. Two of these three different reconstructions have been observed previously also for Fe on Nb(110) [2]. For the pseudomorphic Fe monolayer on Ta(110), we indeed find a spin spiral with a period of roughly 6 nm as the magnetic ground state at zero field.

[1] L. Rózsa *et al.*, Phys. Rev. B, **91**, 144424 (2015) [2] J. Goedecke *et al.*, ACS Nano, **16**, 14066-14074 (2022)

O 50.2 Wed 10:45 REC C 213

Spin polarization in polyalanine molecules: the role of coupling, chirality and coordination — •T. N. Ha Nguyen[1], L. L.T. Baczewski[2], and C. Tegenkamp[1] — [1]Solid Surface Analysis, Technische Universität Chemnitz, Germany — [2]Institute of Physics, Polish Academy of Sciences, Al. Lotnikow, Warszawa, Poland

Propagation of electrons along helical polyalanine-based backbone structures comes along with a robust spin polarization effect. However, studies on a molecular scale are still rare, although this length scale provides direct insight into the role of molecular properties. The self-assembly process and electronic transmission properties of race- mats of right and left handed *-helix polyalanine (DL-PA) molecules from solution on atomically smooth and magnetically switchable Al2O3/Pt/Au/Co/Au substrates was investigated by ambient scan- ning tunneling microscopy and spectroscopy. For various lengths of molecules with and without a cysteine termination, we studied the spin polarization in detail. The phase separation into well-ordered enantiopure hexagonal phases and hetero-dimer structures (DL-PA) allow for the analysis of the spin polarization of PA molecules in different environments. The spin polarization reaches up to 70% for chemisorbed molecules arranged in an hexagonal phase. Our results clearly demonstrate that both the coupling as well as the ordering and coordination are important in order to achieve a high spin-polarization in chiral systems.

O 50.3 Wed 11:00 REC C 213

Robust Monolayers of Endohedral Fullerenes: Towards Highly Ordered Arrays of Single Molecule Magnets and Spin Qubits — •Lukas Spree[1], Luciano Colazzo[1], Caroline Hommel[1], Andreas Heinrich[1], and Alexey Popov[2] — [1]IBS Center for Quantum Nanoscience, Seoul, South Korea — [2]Leibnitz Institute for Solid State and Materials Research

In 2012 DySc$_2$N@C$_{80}$ was the first endohedral fullerene proven to be a single molecule magnet. Ten years and many fullerene based single molecule magnets later, lanthanide dimetal fullerenes show high blocking temperatures of magnetization approaching 30 K and suppression of quantum tunnelling of magnetization at zero magnetic field due to coupling of two magnetic moments via an electron in a singly occupied molecular orbital. The isostructural non-magnetic versions of these molecules with Y or Sc dimers show long T$_2$ times and might be promising candidates for spin qubits. A great advantage of fullerene based molecules is their exceptional chemical stability.

For future research the deposition of fullerene based single molecule magnets in ordered layers is desirable to control intermolecular interactions and ease measurements with scanning probe techniques. Several causes for disorder can be identified and one approach to counteract them is chemical functionalization of the fullerene cage to promote self-assembly of monolayers. A challenge with the direct deposition of functionalized fullerenes on a substrate is a mismatch of the distance between potential binding sites and the size of the fullerenes. Therefore, templating with tetrapyrrole complexes is investigated.

O 50.4 Wed 11:15 REC C 213

Tuning the magnetic properties of self-assembled molecular networks on Au(111) and graphene — •Adam J. Watson, Koen Houtsma, Mihaela Enache, Antonija Grubišić Čabo, and Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, 9747 AG, Groningen, The Netherlands

The ability to manipulate the spin state of low dimensional magnetic networks is of emerging interest and forms the basis of prospective technologies in the atomic limit. These include molecule-based quantum computers and spintronic devices, which require addressable spin architectures. Recently, two-dimensional (2D) networks have been prepared using the methods of on-surface supramolecular self-assembly, exhibiting a variety of different magnetic exchange interactions which are experimentally accessible. [1]

In this work, we performed scanning tunnelling spectroscopy (STS) and x-ray magnetic circular dichroism (XMCD) measurements to characterize the magnetic properties of self-assembled networks of a cyano-functionalized cobalt-porphyrin derivative (CoTCPP) on Au(111) [2] and graphene. Kondo and XMCD measurements indicate a variation in spin-substrate coupling with bonding motif, and variations in magnetic moment and spin distribution. These results highlight the importance of the bonding motif within supramolecular architectures, and the role of the substrate, in tuning molecular magnetism.

[1] Girovsky, J. et al., Nat. Comm. 8 (2017) 15388

[2] B. D. Baker Cortes et al., J. Phys. Chem. C 123 (2019) 19681

O 51: Surface Magnetism

Time: Wednesday 11:30–13:00 Location: REC C 213

O 51.1 Wed 11:30 REC C 213

Turning by hydrogen adsorption an exchange frustrated spin-spiral into elliptical magnetic skyrmions — Timo Knispel[1], Vasily Tseplyaev[2], Markus Hoffmann[2], Gustav Bihlmayer[2], Stefan Blügel[2], Thomas Michely[1], and •Jeison Fischer[1] — [1]II Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Spin-spiral states may emerge either from the frustration of Heisenberg-type exchange interactions or from the competition of exchange and the relativistic Dzyaloshinskii-Moriya interaction resulting in atomic scale and mesoscale textures, respectively. However, to turn frustration-stabilized spin-spirals into skyrmions, high magnetic fields are required, hardly achievable in the lab. We report on a new principle using hydrogen adsorption to unwind an exchange-stabilized spin-spiral into skyrmions at accessible fields. With spin-polarized scanning tunneling microscopy we identify an atomic scale right-handed Néel-type spin spiral on the double layer Fe on Ir(110). Density functional theory calculations confirm the spin spiral is mainly frustration-stabilized with a formation energy of -12 meV/Fe with respect to ferromagnetic state. A field of the order of 80 T would be required to unwind the spin spiral. After adsorption of hydrogen, we observe that the nature of the spin spiral becomes of Dzyaloshinskii-type with a seven times longer period. Elliptical skyrmions can be formed at moderate magnetic fields.

O 51.2 Wed 11:45 REC C 213

Aging in the self-induced spin glass Nd(0001) — •Lorena Niggli, Julian H. Strik, Anand Kamlapure, Mikhail I. Katsnelson, Daniel Wegner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands

Elemental neodymium has been shown to be a self-induced spin glass, where glassy behaviour stems solely from the frustrated nature of the magnetic interactions [1]. This is in contrast to traditional spin glasses, where the presence of disorder is essential toward realizing glassy behaviour. The magnetic state of Nd(0001) is characterized by a lack of long range order, but exhibits local non-collinear order (Q-states). Upon increasing the temperature, neodymium displays an unusual magnetic phase transition from a self-induced spin glass to a long-range ordered multi-Q phase [2]. Here, we explore the aging behaviour of Nd(0001) in its self-induced spin glass state using spin-polarized scanning tunneling microscopy in varying magnetic fields and variable temperature. We explore how the favourability of the Q-states evolves as we age the system and relate these changes to the preferred structure of the ordered phase. These observations indicate that neodymium may be a multi-well system, which deviates from the traditional energy landscape expected of prototypical spin glass systems, thus providing a new platform to study aging dynamics as well as dynamic heterogeneity.

[1] U. Kamber et al., *Science* **368** (2020).

[2] B. Verlhac et al., *Nat. Phys.* **18** (2022).

O 51.3 Wed 12:00 REC C 213

Magnetic Phase Transition in MoS$_2$ detected with AFM — Alexina Ollier[1,2], •Akash Gupta[1], Marcin Kisiel[1], Mehdi Ramezani[1,2], Andreas Baumgartner[1,2], Christian Schönenberger[1,2], and Ernst Meyer[2] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel — [2]Swiss Nanoscience Institute, Klingelbergstrasse 82, CH-4056 Basel

Low doping electron-electron interactions in monolayer MoS$_2$ lead to a ferromagnetic spin order, whereas larger occupation of spin-polarized energy bands results in paramagnetism. The electron density of MoS$_2$ might be tuned with gate voltage, thus providing the switch ability of the ferromagnetic to paramagnetic first-order phase transition. Spontaneous phase transition in two-dimensional semiconductor gated MoS$_2$ monolayer is detected by magnetic force spectroscopy.

An abrupt and reproducible changes of the magnetic force were observed at doping concentration equal to $n_c = 3.0\times10^{12}$ cm^{-2} and are attributed to ferromagnetic to paramagnetic phase change. Linear dependence of force versus external magnetic field was noted in the paramagnetic state, whereas no such dependence was found in already polarised ferromagnetic state. The extracted spin susceptibility confirms the correlated electron system and the observed hysteresis of the measured magnetic force is a strong hint for first-order type of transition.

O 51.4 Wed 12:15 REC C 213

Electron Spin-Polarizing Mechanisms in Chiral CuO and CoO$_x$ Catalyst Surfaces — •Paul Valerian Möllers[1], Jimeng Wei[2], Supriya Ghosh[2], Soma Salamon[3], Manfred Bartsch[1], Heiko Wende[3], David Waldeck[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, WWU Münster, Germany — [2]Department of Chemistry, University of Pittsburgh, Pittsburgh, USA — [3]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), Universität Duisburg-Essen, Germany

Spin-polarized catalytic surfaces can greatly enhance the selectivity of chemical reactions, e.g., in a photoinduced water splitting process. Here, we present new insights into the mechanisms that give rise to the spin polarization in chiral cupric oxide[1] (CuO) and cobalt oxide[2] (CoO$_x$) layers deposited using a method pioneered by Switzer et al.[3] Photoelectrons were excited with deep-UV laser pulses and their average spin polarization (SP) was measured. For CuO layers, the energy dependence of the spin polarization reveals that the measured SP values can be rationalized assuming an intrinsic SP in the chiral oxide layer and a chirality-induced spin selectivity (CISS)-related spin filtering of the electrons.[4] On chiral CoO$_x$ layers, the SP was found to depend on the Co oxidation state, which allows for reversible switching of the preferred spin orientation. The results support efforts towards a rational design of further spin-selective catalytic oxide materials. [1]K.B. Ghosh et al., *J. Phys. Chem. C* **123**, 3024 (2019) [2]S. Ghosh et al., *J. Phys. Chem. C* **124**, 22610 (2020) [3]Kothari et al., *Chem. Mater.* **16**, 4232 (2004) [4]Möllers et al., *ACS Nano* **16**, 12145 (2022)

O 51.5 Wed 12:30 REC C 213

Magnetic circular dichroism of oxygen-passivated and bare Fe(100) in threshold PEEM — •David Huber[1], Friederike Wührl[1], Maximilian Paleschke[1,2], Frank Schumann[3], Stefan Förster[1], and Wolf Widdra[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Institute of Atomic and Molecular Sciences (IAMS), Academia Sinica, Taipei, Taiwan — [3]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Magnetic circular dichroism (MCD) in threshold PEEM enables imaging of in-plane and out-of-plane oriented ferromagnetic domains in real and momentum space [1, 2]. Here, we compare PEEM and ARPES data for Fe(100) and the oxygen-passivated Fe(100)-(1×1)-O. Imaging the in-plane domains we observe four different asymmetry levels, which we assign to the four magnetization vectors pointing in the high symmetry directions. The observed asymmetry values vary from 3% up to 5,5% comparing Fe(100)-(1×1)-O and Fe(100). The domain-specific momentum space measurements on Fe(100) are thereby in good agreement with relativistic photoemission calculations [2]. Through off-normal photoemission we increase the sensitivity of the method by one order of magnitude in comparison to previous reports [1].

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

[2] Henk and Johansson, J. Electr. Spectr. Relat. Phenom. **94**, 259 (1998).

O 51.6 Wed 12:45 REC C 213

Utilizing symmetry for magnetic domain imaging via PEEM — •Frank O. Schumann[1], Jürgen Henk[2], Maximilian Paleschke[2], Cheng-Tien Chiang[3], and Wolf Widdra[2] — [1]Max-Planck Institut für Mikrostrukturphysik, Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany — [3]Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

It is a well-established fact that the photoemission intensity depends on the polarization state of the light and magnetization direction. For a microscopic description it is vital to include both the spin-orbit and exchange interaction on an equal footing. A photoelectron emission microscope (PEEM) allows the detection of all emitted electrons in the hemisphere. The magnetic contrast is achieved by collecting intensity images with circular polarized light of different helicities. Computing the difference images reveals magnetic domains in the real space imaging mode. In the momentum imaging the angle-resolved photoemission intensity becomes accessible. Symmetry considerations dictate a relation in momentum space of the asymmetry signal from opposite domains. We illustrate these insights by photoemission calculations on an Fe(100) surface for photon energies in the threshold region. These we compare with recent experiments on an Fe(100) surface employing a PEEM in this photon energy range. We discuss the benefit of selecting a window of the momentum of electrons which reach the detector. A careful choice of the allowed momentum range of the detected electrons leads to a selectivity of the magnetization direction of domains.

O 52: Heterogeneous Catalysis and Surface Dynamics I

Time: Wednesday 10:30–12:45 Location: TRE Phy

O 52.1 Wed 10:30 TRE Phy

In-situ spectro-microscopy of single PtRh nanoparticles during oxidation — •Jagrati Dwivedi[1], Lydia Bachmann[1,2], Arno Jeromin[1], Liviu C. Tănase[3], Aarti Tiwari[3], Lucas Caldas[3], Thomas Schmidt[3], Thomas F. Keller[1,2], Beatriz Roldán Cuenya[3], and Andreas Stierle[1,2] — [1]CXNS, Deutsches Elektronen-Synchrotron DESY, D-22607 Hamburg, Germany — [2]Physics Department, University of Hamburg, D-20355 Hamburg, Germany — [3]Department of Interface Science, Fritz-Haber-Institut der Max-Planck Gesellschaft, D-14195 Berlin, Germany

Heterogeneous catalysts are an integral part of industrial scale energy production, conversion and storage. However, a detailed understanding of how their shape, size, structural arrangement and chemical composition affect catalytic activity, selectivity and lifetime remains far from understood. The characterization under catalytic conditions remains challenging, therefore, a spectroscopic analysis of individual PtRh nanoparticles can provide direct evidence of the adsorbed species and their oxidation state. Here, we examined core-shell arranged PtRh nanoparticles on niobium-doped STO single crystals that were achieved by dewetting a homogeneous Pt film and subsequent overgrowth with Rh. Ex situ Scanning Auger Microscopy before and after the oxidation showed that the overgrown Rh is sintering. Spatially resolved in situ X-ray photoemission at BESSY II indicates the formation of Rh_2O_3 at partial oxygen pressure. While the nanoparticles surface composition reflects the oxidation and H_2 reduction, the shape of the nanoparticles remains rather unchanged under the applied conditions.

O 52.2 Wed 10:45 TRE Phy

Probing Au(111) Surface Reconstruction by Electrocatalytic Reactions — •Johannes M. Hermann[1], Areeg Abdelrahman[1], Ludwig A. Kibler[1], and Timo Jacob[1,2,3] — [1]Institute of Electrochemistry, Ulm University, Ulm, Germany. — [2]Helmholtz-Institute-Ulm (HIU), Ulm, Germany. — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany.

Au(111) is an extensively studied single crystal and its thermodynamically most stable surface is reconstructed under UHV conditions. Besides the thermally reconstructed and the unreconstructed Au(111) surfaces, in addition, there is also a potential-induced reconstruction in electrochemical environments. The phase transition between the reconstructed and unreconstructed Au(111) electrode surfaces has mostly been investigated by means of *in situ* scanning tunneling microscopy. Kinetic studies are sparse and in the case of potential-induced reconstruction limited to *in situ* surface X-ray scattering. Since the electrocatalytic hydrogen evolution reaction (HER) on gold electrodes is strongly structure-sensitive, here we show how it can be used to monitor structural changes of the Au(111) surface [1]. The electrocatalytic activity is highest directly after the surface reconstruction had been lifted, and decreases while the potential-induced reconstruction proceeds, following a simple first-order rate law. In contrast to expectations from conventional electrode kinetics, the rate of the reconstruction process decreases with more negative potential, as the reconstructed surface is stabilized by increasing negative excess charge.
[1] J.M. Hermann, *et al.* Electrochim. Acta. **2020**, *347* 136287.

O 52.3 Wed 11:00 TRE Phy

Transition metal carbides vs platinum as catalysts for H2 dissociation and hydrogenation of ethylene and acetylene — •Carlos Jimenez-Orozco[1], Elizabeth Florez[1], and Jose Rodriguez[2] — [1]Faculty of Basic Sciences, University of Medellin, Medellin, Colombia — [2]Chemistry Division, Brookhaven National Laboratory, USA

Hydrogenation reactions are key in the chemical industry, many of them use the scarce Pt-group metals as catalysts, limiting their usage in the long term. Transition metal carbides (TMC) emerge as an alternative material. Among TMC, tungsten carbide (WC) stands out as the active phase or as support of metals. There is still a lack in the understanding of the WC performance, limiting their modulation and applications. Here, density functional theory was used to study the performance of WC in hydrogenation of acetylene (C2H2) and ethylene (C2H4) as probe molecules, together with the H2 dissociation capability of WC. Hence, Pt, Pt/WC (Pt monolayer) and WC were compared. Hydrogen surface coverage and atomistic thermodynamics were used to achieve more realistic models. The H2 dissociation on Pt/WC has a Pt-like behavior at high coverage. The pristine WC surface becomes as a machine for H2 dissociation in a wide rage of T and P, achieving high surface coverages. The Pt/WC has the capability to hydrogenate selectively C2H2 into C2H4, avoiding surface poisoning. The results put WC and Pt/WC under the spotlight as a promising systems alternative to Pt for hydrogenation reactions at several T and P conditions and for the selective transformation of C2H2 into C2H4.

Topical Talk O 52.4 Wed 11:15 TRE Phy

Modeling and Design of Single-Atom Alloy Catalysts — Raffaele Cheula and •Mie Andersen — Department of Physics and Astronomy, Aarhus University, Denmark

In this contribution we apply molecular simulations and machine learning (ML) to study CO_2 hydrogenation (reverse water-gas shift) on single-atom alloy (SAA) catalysts, i.e., diluted bimetallic materials. SAAs have been shown to be able to break the scaling relationships that limit conventional catalysts [1]. We target a wide combinatorial space of elements of the periodic table, which makes a direct study with density-functional theory (DFT) computationally prohibitive. Therefore, we produce a database of DFT-calculated energies on a limited number of SAAs and apply physics-inspired ML techniques for the extrapolation to a wide range of materials. We use a graph-based Gaussian Process Regression ML model (WWL-GPR [2]) to calculate adsorption energies, and simpler models (e.g., multivariate regressions) to estimate the activation energies of the new materials. We employ microkinetic modeling to simulate the reaction kinetics; then, we apply sensitivity analysis and uncertainty quantification to identify the parameters that can improve the model predictions, and we refine them with additional DFT calculations. The application of the framework to CO_2 hydrogenation allows us to rationalize how reaction mechanisms and catalytic activity change with the catalyst composition, paving the way toward the design and nano-engineering of SAA catalysts.

[1] RT. Hannagan *et al.*, Chem. Rev. **120**, 12044 (2020)
[2] W. Xu *et al.*, Nat. Comp. Sci. **2**, 443 (2022)

O 52.5 Wed 11:45 TRE Phy

Data-centric approach for uncovering rules to describe the CO_2 activation at metal catalysts — •Herzain I. Rivera-Arrieta, Lucas Foppa, and Matthias Scheffler — The NOMAD Laboratory at the Fritz-Haber-Institut der Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin, Germany

Using CO_2 as a building block in the production of chemicals and fuels requires, in a first step, the activation of this molecule [1]. The materials space is practically infinite, but only a handful of them may enable an effective CO_2 activation. Therefore, this work focuses on the use of artificial intelligence to speed up finding new catalysts for this process. Single-atom alloys (SAA) of transition metals not only provide good model systems, but also show potential as heterogeneous catalysts [2]. Using the mBEEF functional to perform the DFT modeling of the interaction between CO_2 and different surface terminations in Cu-, Zn-, and Pd-based SAA, we generated a dataset including 50 physicochemical parameters characterizing the geometry, and electronic properties of the adsorption sites where the molecule is activated in each material. Then, we applied the subgroup-discovery (SGD) approach [3] to

uncover rules correlating key parameters in the SAA with indicators of the CO_2 activation, e.g., a large C−O bond elongation. Having access to these SGD-rules, which only depend on the material, allows a fast screening and prediction of potentially effective catalysts.
[1] H. J. Freund and M. W. Roberts, *Surf. Sci. Rep.*, **25**, 225 (1996).
[2] J. Schumann, *et al.*, *J. Phys. Chem. Lett.*, **12**, 10060 (2021).
[3] B. R. Goldsmith, *et al.*, *New J. Phys.*, **19**, 013031 (2017).

O 52.6 Wed 12:00 TRE Phy

Machine learning interatomic potential for metallic and oxidized copper surfaces — •Felix Riccius, Nicolas Bergmann, Nicolas G. Hörmann, Hendrik H. Heenen, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

Copper (Cu) is a promising catalyst for the electrochemical reduction of CO_2 to chemicals and fuels since it yields many possible reduction products. The selectivity between these products is hypothesized to be altered by partial oxidation of the catalysts* surface. The extent of Cu surface oxidation, as well as accompanying morphological transformations are, however, unclear. Predictive atomistic simulations could potentially uncover this surface chemistry but time and length scales necessary for the required sampling are intractable by first-principles methods. Machine learning interatomic potentials (MLIP) trained to first principle data can overcome this limitation by retaining predictive accuracy at a fraction of the computational cost. In this work, we use Gaussian Approximation Potentials to train a MLIP for metallic Cu and Cu oxides. We design a workflow tailored to the problem at hand. Via iterative parallel tempering simulations, we sample the relevant phase space for Cu oxidation at various oxidation states during training. We demonstrate the viability of our approach, which results in a reliable potential capable of describing the chemically important regions of the configuration space. The potential gives access to (surface)phase diagrams and surface reconstruction phenomena following surface reduction and oxidation. The atomic insight may shine light on the role of (surface)oxidation in Cu electrocatalysts.

O 52.7 Wed 12:15 TRE Phy

Selectivity Trends and Role of Adsorbate–Adsorbate Interactions in CO Hydrogenation on Rhodium Catalysts — •Martin Deimel[1,2], Hector Prats[3], Michael Seibt[2], Karsten Reuter[1], and Mie Andersen[4] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Chair for Theoretical Chemistry, Technical University of Munich, Germany — [3]Department of Chemical Engineering, University College London, UK — [4]Aarhus Institute of Advanced Studies and Department of Physics and Astronomy, Aarhus University, Denmark

Rh is one of the most promising elemental catalysts for the conversion of syngas (CO and H_2) into hydrocarbons and oxygenates, especially toward valuable higher oxygenates. Experimentally, an inverse relationship between activity and selectivity of the main products methane and acetaldehyde was identified with conflicting explanations for this trend.[1,2] Here, we revisit the question of the role played by step and terrace sites, represented by the Rh(211) and Rh(111) facets, on activity and selectivity trends.[3] We use an accelerated kinetic Monte Carlo (KMC) approach including a cluster expansion to treat lateral interactions. By comparing our results to corresponding mean-field models and experiment,[1,2] we find that only the KMC models can correctly capture the experimental selectivity trends and that quantitatively correct activity predictions require correction for well-known errors in the density functional theory parametrization of our models.
[1] N. Yang *et al.*, J. Am. Chem. Soc. **138**, 3705 (2016)
[2] M. Schumann *et al.*, ACS Catal. **11**, 5189 (2021)
[3] M. Deimel *et al.*, ACS Catal. **12**, 7907 (2022)

O 52.8 Wed 12:30 TRE Phy

Estimating Free Energy Barriers for Heterogeneous Catalytic Reactions with Machine Learning Potentials and Umbrella Sampling — •Sina Stocker[1], Gábor Csányi[2], Karsten Reuter[1], and Johannes T. Margraf[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]University of Cambridge, United Kingdom

Predictive-quality first-principles based microkinetic models are increasingly used to analyze (and subsequently optimize) reaction mechanisms in heterogeneous catalysis. In full rigor, such models require the knowledge of all possible elementary reaction steps and their corresponding reaction barriers. Unfortunately, for complex catalytic processes (such as the generation of ethanol from syngas) the number of possible steps is so large that an exhaustive first-principles calculation of all barriers becomes prohibitively expensive.

To overcome this limitation, we develop machine learned (ML) interatomic potentials to model the early steps of syngas conversion on Rhodium. These ML potentials can be used to determine free energy reaction barriers at a fraction of the computational cost of the underlying first-principles method. Specifically, we use here the Gaussian Approximation Potential (GAP) framework and explore iterative training in combination with umbrella sampling for the CHO decomposition as an example.

O 53: Focus Session: Frontiers of Electronic-Structure Theory IV (joint session O/HL)

Time: Wednesday 10:30–13:00 Location: TRE Ma

O 53.1 Wed 10:30 TRE Ma

A systematic DFT+U and Quantum Monte Carlo benchmark of magnetic two-dimensional (2D) CrX_3 (X = I, Br, Cl, F) — •Daniel Wines, Kamal Choudhary, and Francesca Tavazza — Materials Science and Engineering Division, National Institute of Standards and Technology (NIST), Gaithersburg, MD 20899, USA

The search for two-dimensional (2D) magnetic materials has attracted a great deal of attention because of the experimental synthesis of 2D CrI_3, which has a measured Curie temperature of 45 K. Often times, these monolayers have a higher degree of electron correlation and require more sophisticated methods beyond density functional theory (DFT). Diffusion Monte Carlo (DMC) is a correlated electronic structure method that has been demonstrated successful for a wide variety of systems, since it has a weaker dependence on the Hubbard parameter (U) and density functional. In this study we designed a workflow that combines DFT+U and DMC in order to treat 2D correlated magnetic systems. We chose monolayer CrX_3 (X = I, Br, Cl, F), with a stronger focus on CrI_3 and $CrBr_3$, as a case study due to the fact that they have been experimentally realized and have a finite critical temperature. With this DFT+U and DMC workflow and the analytical method of Torelli and Olsen, we estimated an upper bound of 43.56 K for the T_c of CrI_3 and 20.78 K for the T_c of $CrBr_3$, in addition to analyzing the spin densities and magnetic properties with DMC and DFT+U. We expect that running this workflow for a well-known material class will aid in the future discovery and characterization of lesser known and more complex correlated 2D magnetic materials.

Topical Talk O 53.2 Wed 10:45 TRE Ma

TREX: an integrated HPC software platform for quantum Monte Carlo calculations — •Claudia Filippi — University of Twente, Enschede, The Netherlands

I will present the software development strategy and current achievements of the European Center of Excellence TREX "Targeting Real chemical accuracy at the EXascale" [1]. TREX focuses on methods at the high-end in the accuracy ladder of electronic structure approaches and, in particular, on quantum Monte Carlo methods which are uniquely positioned to fully exploit the massive parallelism of upcoming architectures. The main objective of TREX is the development of a user-friendly and open-source software suite, which integrates quantum Monte Carlo codes within an interoperable, high-performance platform. Core of our software efforts is the creation of the following two libraries:

- TREXIO: A common I/O library and file format for easily exchanging data between applications, facilitating high-throughput computing workflows [2];
- QMCkl: A library of computational kernels, written together by quantum Monte Carlo and HPC experts, to perform common CPU-intensive quantum Monte Carlo tasks [3].

[1] https://trex-coe.eu
[2] https://github.com/trex-coe/trexio
[3] https://trex-coe.github.io/qmckl

O 53.3 Wed 11:15 TRE Ma

Exciton-phonon coupling in luminescence of indirect band-gap materials — Matteo Zanfrognini[1,2], Fulvio Paleari[1], Daniele Varsano[1], and •Ludger Wirtz[3] — [1]Centro S3, CNR-Istituto Nanoscienze, Modena, Italy — [2]Università di Modena e Reggio Emilia, Modena, Italy — [3]Department of Physics and Materials Science, University of Luxembourg, Luxembourg

Layered, quasi-2D materials, such as hexagonal boron nitride (hBN) are known to display very strong excitonic effects due to the concentration of excitons in two dimensions and due to the relatively weak dielectric screening. If the band-gap of the material is indirect, the dispersion of the lowest lying exciton can have a minimum at a finite wave vector q. Upon absorption of a photon and excitation to a vertical (q=0) exciton, the system will relax to the finite-q exciton. Luminescence then entails the absorption/emission of a phonon with wave vector q. We present a computational approach for phonon-assisted luminescence in the presence of strong excitonic effects using two approaches: (i) a finite-displacement approach for the exciton-phonon coupling and (ii) a diagrammatic approach, calculating the q-dependent exciton-phonon coupling from the exciton eigenvectors and electron/hole-phonon scattering matrix elements. We show that the methodology quantitatively explains recent measurements of different stackings of BN layers. [1]

[1] A. Plaud, I. Stenger, F. Fossard, L. Sponza, L. Schué, F. Ducastelle, A. Loiseau, J. Barjon, to be published.

O 53.4 Wed 11:30 TRE Ma

A combined G_0W_0/BSE scheme of characterizing photoexcitations in hydroxylated rutile TiO_2(110) — •Savio Laricchia, Andrea Ferretti, Daniele Varsano, and Claudia Cardoso — Centro S3, CNR-Istituto Nanoscienze, 41125 Modena, Italy

In reduced TiO_2, electronic transitions originating from polaronic excess electrons in surface-localized band-gap sta tes (BGS) are known to contribute to the photoabsorption and to the photocatalytic response of TiO_2 in the visible region. Recent state-selective studies using two-photon photoemission (2PPE) spectroscopy have also identified an alternative photoexcitation mechanism contributing to the photoabsorption of the reduced surface (110) of rutile TiO_2. This process involves *d-d* excitations from BGS arising from surface and subsurface defects, including bridging hydroxyls and oxygen vacancies. Density Functional Theory (DFT) has been used to determine the character of the electronic excited states involved in a $d_{t_{2g}}$-$d_{t_{2g}}$ transitions, but its accuracy is questioned by its theoretical framework: DFT is in principle exact for ground state systems and does not describe interacting photogenerated electron-hole pairs, i.e. the excitons. This has highlighted the need to move beyond the DFT formalism, by working within a many-body perturbation theory (MBPT) framework. It will be shown how a G_0W_0 method, combined with the solution of the Bethe-Salpeter equation (BSE), provides a powerful tool for characterizing from first principles the optical excitations from BGS identified by 2PPE experiments on hydroxylated TiO_2(110).

15 min. break

O 53.5 Wed 12:00 TRE Ma

Scaling the Way for All-Electron XPS Simulations to CalculateAbsolute Binding Energies of Surface Superstructures — •Dylan Morgan[1], Sam Hall[1], Benedikt Klein[1,2], Matthew Stoodley[1,2], and Reinhard Maurer[1] — [1]Department of Chemistry, University of Warwick, United Kingdom — [2]Diamond Light Source, Harwell Science and Innovation Campus, United Kingdom

First principles simulations of x-ray photoemission spectroscopy (XPS) and near-edge x-ray absorption fine-structure (NEXAFS) crucially support the assignment of surface spectra composed of many overlapping signatures. Core-level constrained Density Functional Theory calculations based on the Δ-SCF method are commonly used to predict relative XPS binding energy (BE) shifts but often fail to predict absolute BEs. The all-electron numeric atomic orbital code FHI-aims enables an accurate prediction of absolute BEs, but the legacy code lacked computational scalability to address large systems and robustness with respect to localisation of the core hole. We present a redesign of the core-hole constrained code in FHI-aims that delivers improvements to the scalability and robustness of core-hole constrained calculations in FHI-aims. We demonstrate the improved scaling behaviour and employ the new code to simulate core-level spectroscopic fingerprints of graphene moire superstructures. The code refactorisation forms the basis to expand the code towards improved core hole localisation methods and the rigorous treatment of relativistic effects for core-level spectra beyond the 1s shell.

O 53.6 Wed 12:15 TRE Ma

Efficient diagonalization of BSE electron-hole Hamiltonian using group theory — •Jörn Stöhler[1,2], Dmitrii Nabok[1], Stefan Blügel[1], and Christoph Friedrich[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [2]RWTH Aachen University, Germany

The Bethe-Salpeter equation (BSE) is the state-of-the-art method for the calculation of optical absorption and electron-energy loss spectra including excitonic effects. We solve the BSE by diagonalizing an effective electron-hole Hamiltonian. Often, a high number of **k**-points is needed to converge the BSE spectra, which leads to a large size of the Hamiltonian matrix and makes its diagonalization very expensive. In this work [1], we use the full spatial symmetry group to transform the electron-hole product basis into a symmetry-adapted product basis, which brings the Hamiltonian into a block-diagonal form and speeds up the subsequent diagonalization. The basis transformation is sparse and causes little overhead. We provide an implementation of our method in the FLAPW code `Spex` and demonstrate speedups of 36, 52, 12 for Si, BN, and monolayer MoS_2, respectively.

We acknowledge financial support by MaX CoE funded by the EU through H2020-INFRAEDI-2018 (project: GA 824143).

[1] J. Stöhler, C. Friedrich, *Unpublished*

O 53.7 Wed 12:30 TRE Ma

Excitonic effects on quadratic optical photoresponse tensors of semiconductors — •Peio Garcia-Goricelaya[1] and Julen Ibañez-Azpiroz[1,2] — [1]Centro de Física de Materiales, University of the Basque Country UPV/EHU, Spain — [2]IKERBASQUE Basque Foundation for Science, Spain

We present a general ab initio scheme for including many-body excitonic effects in the non-linear optical photoresponse up to second order. Our practical implementation starts from the length-gauge formulation of the single-particle non-interacting optical photoresponse tensors [1] that are efficiently calculated using Wannier interpolation [2]. Subsequently, excitonic corrections are included in the many-body interacting current-density response tensors by means of Dyson-like equations derived within TD-CDFT. These equations allow a natural connection with the formalism of the single-particle picture and the Wannier-interpolation scheme respecting the tensorial character of the response. We employ this scheme to assess the impact of excitonic effects on several quadratic optical processes as the second-harmonic generation and the shift-current bulk photovoltaic effect in technologically appealing semiconductors.

Funding provided by the European Union*s Horizon 2020 research and innovation programme under the European Research Council(ERC) grant agreement No 946629.

[1] J. E. Sipe and A. I. Shkrebtii, Phys. Rev. B 61, 5337 (2000).

[2] G. Pizzi et al., J. Phys. Cond.Matt. 32, 165902 (2020)

O 53.8 Wed 12:45 TRE Ma

Electronic and optical properties of $CoFe_2O_4$ from density functional theory calculations, including many-body effects — •Shohreh Rafiezadeh[1], Vijaya Begum-Hudde[1,2], and Rossitza Pentcheva[1] — [1]Department of Physics University of Duisburg-Essen, Germany — [2]University of Illinois at Urbana-Champaign, USA

$CoFe_2O_4$ is a ferrimagnetic semiconductor that finds application as an anode material in photocatalytic water splitting. We present a comprehensive study of the electronic and optical properties of bulk $CoFe_2O_4$ using density functional theory calculations and many-body perturbation theory to clarify the broad range of reported band gaps both experimentally (0.55-4.1 eV)[1] and theoretically (0.9-1.90 eV). Starting with different exchange-correlation functionals, we obtain a direct band gap of 1.38 [PBE+(U=4 eV)], 1.69 eV [SCAN+(U=3 eV)], and an indirect gap of 2.02 eV (HSE06). Including quasiparticle corrections within G_0W_0 enhances and renders indirect band gaps for all functionals of 1.78, 1.95 and 2.17 eV, respectively. Excitonic effects are accounted for by solving the Bethe Salpeter equation and result in the lowest threshold for optical transitions at 1.50 eV (SCAN) and 1.61 eV (HSE06), followed by peaks at $\sim$ 2.0, 3.5 and 5.0 eV, in agreement with experiment highlighting the importance of electron-hole interactions. Support by DFG- within CRC/TRR 247, project B04, and computational time at MagnitUDE is gratefully acknowledged. [1] S. Singh and N. Khare, Sci. Rep. **8**, 6522 (2018).

O 54: Focus Session: Scanning Probe Microscopy with Quartz Sensors II

Time: Wednesday 15:00–17:30 Location: CHE 89

Topical Talk O 54.1 Wed 15:00 CHE 89

Peering into interfacial water by qPlus-based atomic force microscopy — •Ying Jiang — International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, P. R. China

Water/solid interfaces are a central theme across an incredibly broad range of scientific and technological processes. Scanning probe microscopy (SPM) has been extensively applied to probe interfacial water, but there exist two longstanding limitations in the past decades, which makes SPM fall short compared with conventional spectroscopic methods. First, it is very difficult to image H atoms of water molecule directly; Second, it is highly possible to disturb the fragile H-bonding water structure during the imaging process. To this end, we have developed a new imaging method based on qPlus-type atomic force microscopy (AFM), which is sensitive to H and non-invasive to water structure. The key lies in probing the high-order electrostatic force between the quadrupole-like CO-terminated tip and the polar water molecules at large tip-water distances. In this talk, I will showcase the application of this technique to probe water clusters, ion hydrates, 2D ice and even bulk ice surface [1-4]. The possibility of combing qPlus-AFM with quantum sensing technology to perform nanoscale NMR measurement of interfacial water will be also briefly discussed [5-6].

[1] Nature Commun. 9, 122 (2018) [2] Nature 557, 701 (2018) [3] Nature 577, 60 (2020) [4] Science 377, 315 (2022) [5] Nature Commun. 12, 2457 (2021) [6] Nature Physics 18, 1317 (2022)

O 54.2 Wed 15:30 CHE 89

Does surface adsorption change the reactivity of an organic molecule? — Jack Henry, Philip Blowey, and •Adam Sweetman — University of Leeds, United Kingdom

Adsorption onto metal surfaces is known to alter the electronic [1], and geometric [2] structure of small organic molecules. However, the change in reactivity of a single molecule induced by the presence of a surface is less well studied. We investigated the influence of molecule-substrate bonding on the interactions experienced by a scanning probe microscope (SPM) tip by studying C60 molecules adsorbed in different configurations [3-5] on the Cu(111) surface, using qPlus NC-AFM/STM at 5K. We compare the minima in collected force spectra to complementary ab initio (DFT) simulations, and discuss the substantial differences in our results compared to the existing literature [3]. 1. Repp, J., et al. (2005). Physical Review Letters, 94(2), 026803. 2. L. Gross, et al. Science 325, 1110 (2009). 3. Jonathan Brand et al. Nano Letters 2019 19 (11), 7845-7851 4. W. W. Pai, et al. Physical Review Letters 104, (2010). 5. L. Forcieri, et al. Physical Review B 104, (2021).

O 54.3 Wed 15:45 CHE 89

Water Dimer-Driven DNA Base Superstructure with Mismatched Hydrogen Bonding — Shuning Cai[1], Lauri Kurki[1], •Chen Xu[1], Adam S. Adam[1,2], and Peter Liljeroth[1] — [1]Department of Applied Physics, Aalto University, 00076 Aalto, Espoo, Finland — [2]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

The existence of water dimers in equilibrium water vapor at room temperature and their anomalous properties revealed by recent studies suggest the benchmark role of water dimers in both experiments and theory. However, there have been limited observations of individual water dimers due to the challenge of water separation and generation at the single-molecule level. Here, we achieve real-space imaging of individual confined water dimers embedded inside a self-assembled layer of a DNA base, adenine, on Ag(111). The hydration of the adenine layers by these water dimers causes a local surface chiral inversion in such a way that the neighboring homochiral adenine molecules become heterochiral after hydration, resulting in a mismatched hydrogen-bond pattern between neighboring adenine molecules. Furthermore, theoretical simulation and calculations corroborate the mutual influence between the adenine superstructure and these dynamic confined water dimers. The observation of single confined water dimers offers an unprecedented approach to studying the fundamental forms of water clusters and their interaction with the local chemical environment.

O 54.4 Wed 16:00 CHE 89

Nanosacle 3D printing technique by using the nanopipette-combined quartz tuning fork-atomic force microscope — •Sangmin An — Department of Physics, Institute of Photonics and Information Technology, Jeonbuk National University, Jeonju 54896, South Korea

Materials can be classified by hardness, such as gold represented by hard materials having elasticity and water represented by soft materials having viscosity. However, at the nanoscale, even solid gold exhibits viscosity [1], while liquid water also exhibits elasticity [2] revealed by a quartz tuning fork-atomic force microscope (QTF-AFM), which has the intrinsic properties of high stiffness and high sensitivity. In this presentation, I discuss how this QTF-AFM can be applied as the nanoscale 3D printing technique combined with nanopipette [3,4], which are typically used in biotechnology, along with showing the results of the elasticity and viscosity of water. In addition, I share the results of nanoscratching [5] and nanosensor [6] schemes which can be realized with the nanorod-combined QTF-AFM instead of nanopipette.

[1] Nature 569, 393-397 (2019).
[2] Phys. Rev. X 8, 041046 (2018).
[3] Nano-Micro Lett. 14, 13 (2022).
[4] Nanoscale Adv. in press (2022).
[5] Appl. Nanosci. 9, 67-76 (2019).
[6] Proc. Natl. Acad. Sci. USA 115(12), 2884-2889 (2018).

Topical Talk O 54.5 Wed 16:15 CHE 89

AFM with the qPlus sensor: An indeal tool for oxide surface science — •Ulrike Diebold — Institute of Applied Physics, TU Wien, Vienna, Austria

The past decades have seen a sustained interest in the atomic-scale properties of metal oxide surfaces. Local probes are well suited to study surface reconstructions, (point) defects, trapped local charges, and the adsorption of small molecules. Much of the work has focused on semiconducting or (ultra-)thin film samples, as these have sufficient conductivity for STM investigations. The superior resolution afforded by the qPlus sensor allows for extending such studies to highly insulating oxides, such as silicates or other minerals. In the talk, I will give an overview of recent progress, fascinating opportunities, and challenges of atomically-resolved AFM on oxides.

O 54.6 Wed 16:45 CHE 89

Atomic-scale imaging of muscovite mica and its interaction with water — •Giada Franceschi[1], Pavel Kocan[2], Andrea Conti[1], Sebastian Brandstetter[1], Jan Balajka[1], Igor Sokolovic[1], Jiri Pavelec[1], Markus Valtiner[1], Martin Setvin[2], Florian Mittendorfer[1], Michael Schmid[1], and Ulrike Diebold[1] — [1]Inst. Appl. Phys., TU Wien, Wiedner Hauptstr. 8-10/E134, 1040 Vienna, Austria — [2]Dept. Surface and Plasma Phys., Charles University in Prague, V Holesovickach 2, 180 00 Prague, Czech Republic

Muscovite mica is an abundant potassium aluminosilicate enjoying wide popularity in surface and interfacial science. Its prevalence is partly due to its extraordinary cleaving properties: The easily obtained atomically flat terraces are ideal for fundamental studies. To date, it is established that the cleaved surface is decorated by K$^+$ ions,[1] but their intrinsic ordering and their precise hydration mechanisms are not known. Here, we use non-contact atomic force microscopy to image the K$^+$ distribution of cleaved mica and investigate their interaction with water under ultra-high vacuum conditions. After cleaving, the ions are arranged with short-range order, which we interpret with support from theory.[2] Dosing water vapor at 100 K causes various hydration arrangements, consistent with previous theoretical studies, and clustering at increasing water coverage. Exposure to ultra-clean liquid water[3] induces ion mobility and substitution by protons. *[1] Christenson et al., Surf. Sci. Reports 71, 367 (2016). [2] Franceschi et al., submitted. [3] Balajka et al., Rev. Sci. Instrum. 89, 083906 (2018)*

O 54.7 Wed 17:00 CHE 89

Surface structure of dry and hydrated α-Al$_2$O$_3$(0001) — Johanna Hütner[1], David Kugler[1,2], Michael Schmid[1], Ulrike Diebold[1], and •Jan Balajka[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]CEITEC, Brno, Czech Republic

Corundum α-Al$_2$O$_3$ is an important ceramic also widely used as a support for heterogeneous catalysis. Due to similar Al coordination, α-Al_2O_3 is an important model system for naturally occurring minerals, such as aluminosilicate clays. Detailed studies of alumina surfaces have been stymied by its insulating nature but successfully performed with atomic force microscopy [1]. We used noncontact AFM to investigate the $(\sqrt{31}\times\sqrt{31})R9^\circ$-reconstructed $Al_2O_3(0001)$ surface formed upon high-temperature annealing. The reactivity of surface sites is strongly affected by hydroxylation. However, complete surface hydroxylation requires high pressures of water vapor (1 Torr) [2] that cannot be easily achieved in a conventional ultrahigh vacuum system. We explored the interaction of the $Al_2O_3(0001)$ surface with varying pressures of water vapor as well as ultrapure liquid water dosed with a UHV-compatible dispenser [3]. The results will provide new insights into the hydration of environmental substrates. [1] J. V. Lauritsen, et al., *Phys. Rev. Lett.* 103, 076103 (2009) [2] P. J. Eng, et al., *Science* 288, 1029 (2000) [3] J. Balajka, et al., *Rev. Sci. Instrum.* 89, 8, 083906 (2018)

O 54.8 Wed 17:15 CHE 89

Atomic-scale imaging of the cleaved feldspar microcline (001) surface and its interaction with water — •Luca Lezuo, Andrea Conti, Jan Balajka, Igor Sokolović, Florian Mittendorfer, Michael Schmid, Ulrike Diebold, and Giada Franceschi — Institute of Applied Physics, TU Wien, Wiedner Hauptstrasse 8-10/E134, 1040 Wien, Austria

Feldspar microcline ($KAlSi_3O_8$), abundant in the Earth's crust and present as dust particles in the atmosphere, is known to be one of the best ice nucleators. The exact processes driving the interaction of microcline with water have been studied intensively [1], but atomic-scale investigations remain elusive.

We present experimental, atomic-scale studies of the microcline-water interaction. The surfaces were prepared by UHV cleaving and analysed with non-contact atomic force microscopy (nc-AFM) and x-ray photoelectron spectroscopy (XPS). The cleaved surface consists of a honeycomb array that we assign to differently back-bonded O atoms. Dosing water vapour at 100 K causes the appearance of a hexagonal lattice and the gradual formation of a connected water network. DFT calculations help us to rationalize our experimental results.

[1] A. Kumar, et al., Atmos. Chem. Phys. 18, 7057 (2018)

O 55: Organic Molecules on Inorganic Substrates IV: Adsorption and Growth II

Time: Wednesday 15:00–17:45 Location: CHE 91

O 55.1 Wed 15:00 CHE 91

Bias-dependent conductivity switching and rectification in metallocene-based molecular junctions — Yangbiao Liu[1], Andika Asyuda[1], Heinrich Lang[2], Egbert Zojer[3], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Fakultät für Naturwissenschaften, Anorganische Chemie, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [3]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, 8010 Graz, Austria

Self-assembled monolayers (SAMs) of ferrocenyl/ruthenocenyl-substituted biphenylthiolates and fluorenethiolates on Au(111) exhibit two distinct conductance states (CS) in two-terminal junctions featuring a sharp tip of eutectic GaIn as top electrode. When only negatively biasing the junction, the original, high CS is preserved, while the junction is switched to a low CS when applying only positive biases. Comparing the current values for these two states, one gets an effective rectification ratio of more than 1000 - a value comparable to the best performing molecular diodes but attained already at particularly low voltages. Significantly, the switching between the conduction states is reversible and the initial, high CS can be recovered by the application of a negative bias. Moreover, as shown by the example of one of the SAMs studied, when sweeping the junction alternatingly to the maximum positive and negative bias voltages (as usually done in literature), fully symmetric J-V curves are observed. This means that for a symmetric sweeping of the junction, the effective rectification disappears.

O 55.2 Wed 15:15 CHE 91

Sensing properties of cerium oxide as an electrode material for the detection of glucose — •Anastasiia Deineko[1], Viacheslav Kalinovych[1], Sascha L. Mehl[2], Yevheniia Lobko[1], Yurii Yakovlev[1], Tomáš Skála[1], Kevin C. Prince[2], Vladimír Matolín[1], Iva Matolínová[1], and Nataliya Tsud[1] — [1]Charles University, Faculty of Mathematics and Physics, Department of Surface and Plasma Science, Prague, Czech Republic — [2]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Trieste, Italy

Detection of glucose level in biological liquids is of great importance nowadays because of the growing number of people with diabetes. A variety of oxides is used as electrode material for biosensors and cerium oxide is among them due to its unique properties. In this study characterization of the cerium oxide was performed by surface analysis techniques using photoelectron and absorption spectroscopies (XPS, SRPES, RPES, NEXAFS) in combination with electrochemical measurements. Photoemission based analysis provided information on changes in the oxidation state of cerium cations on the surface and in the subsurface layers of the oxide film, and whether glucose chemically bonds to the oxide. While electrochemical testing, namely cyclic voltammetry and chronoamperometry, was used to explore the sensing properties of polycrystalline cerium oxide films in reaction with glucose in the PBS working solution. The CeO_2 working electrode sensitivity and pH range of sensor stability were determined and discussed in view of the enzymatic properties of cerium oxide. Keywords: cerium oxide, glucose, photoelectron spectroscopy, electrochemistry, biosensor.

O 55.3 Wed 15:30 CHE 91

Exploiting Cooperative Catalysis for the On-Surface Synthesis of Linear Heteroaromatic Polymers via Selective C-H Activation — Xunshan Liu[1], Adam Matej[2,3], Tim Kratky[4], Jesús I. Mendieta-Moreno[2], Sebastian Günther[4], Pingo Mutombo[2], Silvio Decurtins[1], Ulrich Aschauer[1], Jascha Repp[5], Pavel Jelinek[2,3], Shi-Xia Liu[1], and •Laerte L. Patera[4,5,6] — [1]Department of Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern, Bern, Switzerland — [2]Institute of Physics of Czech Academy of Sciences, Prague, Czech Republic — [3]Regional Centre of Advanced Technologies and Materials, Palacký University Olomouc, Olomouc, Czech Republic — [4]Department of Chemistry, Technical University of Munich, Garching, Germany — [5]Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany — [6]Institute of Physical Chemistry, University of Innsbruck, Austria

Regiospecific C-H activation is a promising approach to achieve extended polymers. Herein, selective C-H activation for dehydrogenative C-C couplings of hexaazatriphenylene by Scholl reaction on Ag(111) is reported. By means of low-temperature scanning probe microscopy, we revealed the formation of one-dimensional polymers with a double-chain structure [1]. The growth process is rationalized by density functional theory calculations, pointing out a cooperative catalytic action of Na and Ag adatoms in steering the selective polymerization.

[1] X. Liu, et al., Angew. Chem. Int. Ed. 2013 61.5 (2022): e202112798.

O 55.4 Wed 15:45 CHE 91

PTCDA mediated Ag(111) step reconstruction as precursor to pinwheel phase — •Danyang Liu[1], Aleš Cahlík[1], Carolina A. Marques[1], Jens Oppliger[1], Ruslan Temirov[2,3], and Fabian D. Natterer[1] — [1]Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]University of Cologne, Faculty of Mathematics and Natural Sciences, Institute of Physics II, 50937 Cologne, Germany

PTCDA (3,4,9,10-Perylenetetracarboxylic dianhydride) forming herringbone islands on Ag(111) is the most striking phase and the prototypical metal-supported organic semiconductor. When we co-deposit PTCDA and Ag on Ag(111) at room temperature, we find that prior to their self-assembly into PTCDA herringbone islands, the molecules implant themselves into and reshape the Ag step edges. The PTCDA-decorated-Ag steps are curved and, depending on whether the Ag steps originate from screw dislocations or a terrace, cause steps reconstruction into multilayer high spirals or isolated Ag islands that both exhibit quantum confinement. At higher coverages, the PTCDA decorated steps may nucleate a distinct pinwheel phase that occasionally proceeds to form a metal-organic framework. Annealing to higher temperatures straightens the PTCDA/Ag steps and may grow more pinwheel phase PTCDA patches, showing yet another tuning knob for organometallic surface science.

O 55.5 Wed 16:00 CHE 91

Growth of ordered two-dimensional cobalt phthalocyanine films on a one-dimensional substrate — •Milan Kubicki, Susi Lindner-Franz, Mario Dähne, and Martin Franz — Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany

The formation of self-assembled layers of organic materials on solid surfaces is an important subject because of their possible application in advanced (opto-) electronic devices. While such a formation of self-assembled monolayers is well established on metal surfaces, the growth on silicon surfaces is much less studied.

Using scanning tunneling microscopy (STM) the molecular arrangement of cobalt phthalocyanine (CoPc) molecules on the In-Si(111)-(4×1) surface is studied [1]. CoPc belongs to the transition metal phthalocyanines being a class of organic semiconductors, which has been already employed e.g. in organic light emitting diodes, in organic photovoltaic cells, and in organic field-effect transistors.

Our data demonstrate that for low CoPc coverages the molecules are highly mobile along the In-Si nanowires. By approaching the saturation coverage, the CoPc molecules stabilize each other by forming a highly ordered two-dimensional monolayer. Based on STM observations a structure model with a (4×4) periodicity could be developed, which precisely explains the experimental observations.

[1] M. Kubicki, S. Lindner-Franz, M. Dähne, and M. Franz, Appl. Phys. Lett. **119**, 133105 (2021).

Topical Talk O 55.6 Wed 16:15 CHE 91

Towards Understanding and Controlling On-Surface Reactions and Self-Assembly Mechanisms — •Daniel Ebeling — Institute of Applied Physics, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

The ability to construct organic nanomaterials with atomic precision is the key for applications in molecular electronics as the (opto-)electronic properties of such quantum materials depend on their atomic structure and size. To develop new strategies for synthesizing organic nanomaterials on surfaces, in-depth knowledge about the reaction processes and self-assembly mechanisms is needed. This can be revealed by visualizing the chemical structure and orientation of individual reaction intermediates using bond imaging atomic force microscopy (AFM).

In this presentation, recent results will be discussed that offer an approach for tuning the self-assembly process of halogenated compounds via reversing the binding selectivity of intermolecular halogen bonds. [1] A strategy for building covalent nanostructures one molecule at a time on an inert sodium chloride surface via scanning probe manipulation is also presented. This enables synthesizing elusive covalent nanoarchitectures, studying structural modifications and revealing pathways of intermolecular reactions. [2] Moreover, possibilities for tweaking the bond imaging technique using torsional and flexural higher eigenmodes of qPlus sensors will be illustrated. [3]

[1] J. Tschakert et al. Nature Communications 11, 5630 (2020)
[2] Q. Zhong et al. Nature Chemistry 13, 1133 (2021)
[3] D. Martin-Jimenez et al. Nanoscale 14, 5329 (2022)

O 55.7 Wed 16:45 CHE 91

Molecular orientation of DHTAP on the nanostructured Cu-CuO stripe phase — •Claudia López-Posadas[1], Antony Thomas[2], Thomas Leoni[2], Olivier Siri[2], Conrad Becker[2], and Peter Zeppenfeld[1] — [1]Institute of Experimental Physics, Johannes Kepler University Linz, Altenberger Str. 69, 4040 Linz, Austria — [2]Aix-Marseille University, CNRS, CINaM, UMR 7325, F-13288 Marseille, France

We have studied the preferential adsorption, structure and molecular orientation of 5,14-dihydro-5,7,12,14-tetraazapentacene (DHTAP) layers on the regularly patterned Cu-CuO stripe phase obtained by sub-monolayer oxygen adsorption on the Cu(110) surface. Using Reflectance Difference Spectroscopy (RDS) and Scanning Tunneling Microscopy (STM) we find that the DHTAP molecules preferentially adsorb on the Cu (110) stripes, where they are always lying flat with their long molecular axis aligned parallel to the [-110]-direction. In contrast, on the subsequently covered Cu(110)-(2x1)O stripes, the DHTAP molecules are aligned with their long molecular axis parallel to the [001]-direction. The evolution of the RDS signal allows to monitor the sequential adsorption and orientation of DHTAP during monolayer formation and the subsequent multilayer growth for different oxygen pre-coverages and, hence, different Cu and CuO stripe widths. Interestingly, beyond the first monolayer, the DHTAP molecules adopt a preferential orientation which critically depends on the initial oxygen coverage, revealing the influence of the Cu-CuO stripe width and the possibility to tune the overall optical anisotropy of these films.

O 55.8 Wed 17:00 CHE 91

Oxygen-induced reorientation of organometallic chains on Cu(110) — •Ilias Gazizullin, Christophe Nacci, and Leonhard Grill — Physical Chemistry Department, University of Graz, Heinrichstraße 28, Graz, Austria

The deposition of molecules onto crystalline surfaces allows their investigation at the single-molecule level by scanning tunneling microscopy (STM). It furthermore gives access to the controllable on-surface synthesis of covalent polymers [1]. Here, we have studied dibromo-p-terphenyl molecules on Cu(110) and on the Cu(110)-(2x1)O striped phase under ultra-high vacuum conditions with low-temperature STM.

Previously, the Cu(110)-(2x1)O striped phase was used as a template for the synthesis of organometallic structures having different sizes and shapes depending on the width of copper stripes [2]. The focus of our study is how pre- or post-adsorbed oxygen and annealing, which is necessary for covalent polymerization, affect the molecular adsorption on the surface. It turns out that on the striped phase the molecules form organometallic chains on the copper areas, oriented in at least three surface directions. Increasing the sample temperature from 300 K to 450 K induces a reorientation of the organometallic chains, which occurs due to stabilization of the reoriented OM chains by embedding in the Cu-O phase.

References

[1] L. Grill, S. Hecht, Nature Chemistry 12, 115-130 (2020)
[2] Q. Fan, J. Dai, T. Wang, J. Kuttner, G. Hilt, J. M. Gottfried, and J. Zhu, ACS Nano 3, 3747 (2016)

O 55.9 Wed 17:15 CHE 91

Simulations of 1D Supramolecular Chains on Gold with Explicit Surface–Substrate Interactions — •Krystof Brezina[1,2], Hubert Beck[1], Mariana Rossi[2], and Ondrej Marsalek[1] — [1]Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany

2,5-diaminobenzoquinone-1,4-diimine molecules deposited on Au(111) have been observed in AFM experiments to assemble into 1D hydrogen-bonded chains, which exhibit different geometries and mechanical properties depending on the conditions at the deposition [1]. While a complete explanation of this behavior remains elusive, it is clear that nuclear quantum effects on the hydrogen bonding play an important role. To clarify this effect, we aim at performing path integral molecular dynamics with *ab initio*-quality potentials, in a system that explicitly takes into account molecules and the surface. Here, we discuss the methodological advances needed to generate meaningful training sets for the neural network potentials that substitute the reference *ab initio* method, in particular when a reaction needs to be well described [2]. We show the nature of the relevant proton-transfer *ab initio* potential energy surfaces as well as initial results focusing on the specific effects of the surface on the geometry of the molecules and on the character of the nuclear quantum effects in the chains.

[1] Cahlík A. et al. *ACS Nano* 2021, 15, 6, 10357–10365
[2] Brezina K., Beck H. and Marsalek O. *In preparation* 2022

O 55.10 Wed 17:30 CHE 91

Controlled Formation of Porous 2D Lattices from C_3 Symmetric Ph_6-Me-Tribenzotriquinacene-OAc_3 — •Markus Leisegang[1], Sinem Toksabay[1], Andreas Christ[1], Patrick Härtl[1], Johannes Krebs[1], Todd B. Marder[1], Soumyajyoti Haldar[2], Stefan Heinze[2], Matthias Bode[1], and Anke Krueger[1,3] — [1]Universität Würzburg, Germany — [2]Universität Kiel, Germany — [3]Universität Stuttgart, Germany

The on-surface self-assembly of molecules is a promising approach to control the properties of resulting 2D lattices. Usually, planar molecules are utilized to prepare flat, structurally confined molecular layers, with only a few recent examples of warped precursors [1,2]. However, detailed control of the superstructures is limited thus far. Herein, we report the temperature-controlled self-assembly of a bowl-shaped, acetylated C_3-symmetric hexaphenyl-tribenzotriquinacene derivative on Cu(111). Combining scanning tunneling microscopy (STM) and density functional theory (DFT) confirms the formation of highly differing arrangements starting with π-stacked bowl-to-bowl dimers at low coverage at room temperature via chiral honeycomb structures, an intermediate trigonal superstructure, followed by a fully carbon-based, flattened hexagonal superstructure formed by on-surface deacetylation, which is proposed as a precursor for holey graphene networks with unique defect structures [3].

[1] T. Lohr et al., J. Am. Chem. Soc. 142, 13565 (2020)
[2] J. Urgel et al., J. Am. Chem. Soc. 141, 13158 (2019)
[3] S. Toksabay et al., Chem. Eur. J. 2022, e202203187 (2022)

O 56: 2D Materials III: Growth, Structure and Substrate Interaction II (joint session O/CPP)

Time: Wednesday 15:00–17:30 Location: GER 37

O 56.1 Wed 15:00 GER 37

Te on Pt(111): Structure and Growth of Surface Tellurides and Pt$_x$Te$_y$ Films — Tilman Kisslinger, Alexandra Schewski, Andreas Raabgrund, Hannah Loh, Lutz Hammer, and •M. Alexander Schneider — Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

By LEED-IV, STM and DFT we investigated the tellurization of Pt(111) in UHV. For Te coverages $\Theta < 0.5$ ML surface tellurides are formed. In this coverage regime and after thermal annealing, we find only two well ordered surface telluride structures with (3×3) and (10×10) periodicity, the former was mistaken for a defective PtTe$_2$ film [1]. Our LEED-IV structure analyses determine the atomic structure and show that the Pt(111) surface undergoes massive reconstructions upon reaction with Te.

For $\Theta > 0.5$ ML, compact islands develop which eventually coalesce to a complete platinum telluride layer. Again by LEED-IV analyses we find that the first layer is a Pt$_2$Te$_2$ layer on which as second layer a PtTe$_2$ film can be grown. Both form an overlayer where 7×7 film unit cells lie on 10×10 Pt(111) unit cells. Furthermore, we find that the interface to the Pt(111) bulk still contains the ≈ 0.5 ML Te originally bound in the (10×10) superstructure. Electronic properties of the films determined by STS and implications for the MBE growth of transition metal dichalcogenides by surface tellurization will be discussed.

[1] L. Liu, D. Zemlyanov, and Y.P. Chen, 2D Mater. **8**, 045033 (2021)

O 56.2 Wed 15:15 GER 37

Electronic, chemical and structural properties of ultrathin Ta$_2$NiSe$_5$ flakes — •Kathrin Küster[1], Yuanshan Zhang[1], Dennis Huang[1], Ulrich Starke[1], and Hidenori Takagi[1,2,3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, 70569 Stuttgart, Germany — [3]Department of Physics, University of Tokyo, 113-0033 Tokyo, Japan

The excitonic insulator is a theoretically proposed state of matter wherein a macroscopic condensate of electron-hole pairs, i.e., excitons, spontaneously forms below a transition temperature. The 2D-layered chalcogenide Ta$_2$NiSe$_5$ has arisen as a leading candidate of an excitonic insulator in a bulk crystal. Here we prepared ultrathin films (down to 2 nm) of Ta$_2$NiSe$_5$ and analyzed their structural, electronic and chemical properties with a NanoESCA (Scienta Omicron) on a local scale. Angle-resolved photoelectron spectroscopy (ARPES), X-ray photoelectron spectroscopy (XPS), together with photoelectron emission microscopy (PEEM) and imaging XPS give detailed insight into the thickness dependent properties of the flakes. By exposure to UV-light we observe a contrast change in the PEEM images which is caused by a strong modification of the work function of the flakes, which we tentatively relate to a phase transition of the Ta$_2$NiSe$_5$ flakes.

O 56.3 Wed 15:30 GER 37

Transition from fractal-dendritic to compact islands for the 2D-ferroelectric SnSe on graphene/Ir(111) — Paulus Aleksa, Sammer Iqbal, Muhammad Ali Martuza, Jiaqi Cai, Thais Chagas, Robin Ohmann, and •Carsten Busse — Universität Siegen, Germany

Monolayer islands of the 2D-ferroelectric SnSe have been grown by MBE under UHV conditions using inert and weakly interacting graphene on Ir(111) as the substrate. After deposition at room temperature, fractal-dendritic islands are observed in STM. The preferential growth directions are aligned with high-symmetry directions of the substrate. Upon annealing the islands become more compact. At 560 K they exhbit their equilibrium shape, higher temperatures lead to desoprtion. The equilibrium shape cannot be simply explained by minimization of the number of unsaturated bonds around the perimeter of an island with given area. The model has to be extended to incorporate the polar character of SnSe, leading to island edges that are charged in dependence of their orientation.

O 56.4 Wed 15:45 GER 37

Reaction of submonolayer amounts of Ti and Te on Au(111) — •Andreas Raabgrund, Tilman Kisslinger, Lutz Hammer, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Titanium ditelluride (TiTe$_2$) belongs to the family of layered 2D transition metal dichalcogenides. It achieved a lot of attention due to the emergence of a charge density wave in the single layer limit. Thicker films, however, do not show this transition [1]. Aiming the MBE growth of TiTe$_2$ we investigated the initial growth of titanium telluride structures on Au(111) both structurally and electronically by STM, STS, LEED-IV structural analysis, and DFT. For a Te coverage of 0.4 ML and a Ti coverage of 0.2 ML on Au(111) a chain-like $(5 \times \sqrt{3})_{\mathrm{rect}}$ superstructure is formed. Our LEED-IV best-fit structure with a Pendry R factor of 0.11 (redundancy $\rho = 9.6$) reveals incorporated Ti atoms each of which forms bonds to two Te atoms residing in approximately hollow positions. Our findings regarding the $(5 \times \sqrt{3})_{\mathrm{rect}}$ superstructure disprove the proposed TiTe$_2$ monolayer on Au(111) [2]. STS shows an approximately 0.5 eV (FWHM) wide peak at +1 V which we can correlate to the density of Ti d-states as obtained from DFT.

[1] P. Chen et al., Nat. Commun. **8**, 516 (2017)
[2] Z. Song et al., Chin. Phys. B **102**, 056801 (2019)

O 56.5 Wed 16:00 GER 37

Monolayers of CoCl$_2$ and CoBr$_2$ on Au(111) - Chemical, magnetic and structural investigation — •Samuel Kerschbaumer[1], Sebastien Hadjadj[2], Andrea Aguirre Baños[3], Danilo Longo[3], Wolfgang Kuch[2], José Ignacio Pascual[3], Celia Rogero[1], and Maxim Ilyn[1] — [1]Centro de Fisica de Materiales (CSIC/UPV-EHU), 20018 Donostia-San Sebastian, Spain — [2]Institut für Experimentalphysik, Freie Universität Berlin, 14195 Berlin, Germany — [3]CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastian, Spain

Magnetic 2D materials have gained increasing interest, due to their potential applications. But while many theoretical calculations predict magnetic order in various 2D materials [1], only few have been experimentally measured [2]. A very promising classes of materials are transition metal halides (TMHs), as many of them crystallise in Van der Waals layered structures, making them easily cleavable, while their partially filled d orbitals generate the perfect foundation for magnetic order, further increasing their attractiveness for future nanotechnologies. In this talk chemical, magnetic and structural properties of single-layer CoCl$_2$ and CoBr$_2$ on Au(111) by scanning tunelling microscopy (STM), X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED) and X-ray absorption spectroscopy (XAS/XMCD) will be presented.

[1] Michael A. McGuire, Crystals, 7(5), 121, (2017)
[2] Djuro Bikaljevic et al., ACS Nano, 15, 14985 (2021)

O 56.6 Wed 16:15 GER 37

Structure determination of mono- and few-layers of the 2D-ferroelectric SnSe on graphene on Ir(111) — •Dina Wilks[1], Paulus Aleksa[1], Simon Chung[2], Peter Modregger[1], Dmitri V. Novikov[3], Vedran Vonk[2], Andreas Stierle[2,4], and Carsten Busse[1] — [1]Physics Department, University of Siegen, Germany — [2]Nanolabor Centre for X-ray and Nano Science CXNS, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Germany — [4]Physics Department, University of Hamburg, Germany

For conventional ferroelectrics the critical temperature T_c quickly falls below technically feasible values for very thin films. This is not the case for two-dimensional materials. Theory predicts strong ferroelectricity for group-IV monochalcogenides, where individual layers are puckered sheets with a phosphorene-like structure. For SnSe, stable ferroelectricity of monolayers at room temperature has been shown by controlled microscopic manipulation. Here, we provide the missing structure determination of these monolayers.

We use surface X-ray diffraction to determine the structure of SnSe mono- and few-layers, the influence of the substrate, and the difference in stacking between a few-layered system and the bulk. SnSe films are prepared by MBE using graphene on Ir(111) as an inert and weakly interacting substrate. We observe one phase with three different orientations of monolayer SnSe islands with respect to graphene, while for the few-layered system two phases are found, each with three different orientations. A change in structure with rising temperature for both systems is seen, which hints towards T_c.

O 56.7 Wed 16:30 GER 37

Electronic properties of epitaxially grown monolayer and bilayer VS_2 on Au(111) — •Mikhail Fonin[1], Sabina Simon[1], Felix Förschner[1], Jannik Dornseiff[1], Julia Tesch[1], Elena Voloshina[2], and Yuriy S. Dedkov[2] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Department of Physics, Shanghai University, 99 Shangda Road, 200444 Shanghai, China

Electronic properties of metallic two-dimensional materials can be strongly influenced by the supporting substrates, upon charge transfer or hybridization effects. In this context, suppression of many-body states in metallic transition metal dichalcogenides epitaxially grown on metallic substrates was recently reported [1]. By combination of scanning tunneling microscopy and first principle calculations we study monolayers and bilayers of VS_2 epitaxially grown on Au(111). We investigate the electronic properties of the monolayer and observe a metallic state with the presence of the incommensurate charge density wave state. Going form monolayer to bilayer VS_2, we observe an evolution from the metallic state to an insulating state.

[1] C. E. Enders *et al.,* Phys. Rev. B 94, 081404(R) 2016.

O 56.8 Wed 16:45 GER 37

Vanadium sulphides on graphene on Ir(111): polymorphs, charge density waves, layer dependency — •Camiel van Efferen[1], Joshua Hall[1], Virgínia Boix[2], Tobias Wekking[1], Nikolay Vinogradov[3], Alexei Preobrajenski[3], Jan Knudsen[2], Jeison Fischer[1], Wouter Jolie[1], and Thomas Michely[1] — [1]Universität zu Köln — [2]Lund University — [3]MAX IV Laboratory

Among 2D materials, vanadium based compounds like VS_2 have attracted substantial research interest due to their predicted electronically correlated and magnetic ground states. However, the charge density wave (CDW) in monolayer (ML) VS_2 and VSe_2 competes with predicted magnetic ground states. This has led to new research directions attempting to unlock the magnetic moment of the V atoms, e.g. via defect creation, alloying or the intercalation of atoms between VS_2 layers.

Here, we present a comprehensive X-ray photoemission spectroscopy and scanning tunneling microscopy study of few-layer, quasifreestanding V_4S_7 and V_5S_8 on Gr/Ir(111), which are created via annealing of stoichiometric VS_2. Annealing ML VS_2 without background S pressure removes S atoms from the top layer of VS_2, creating the striped compound V_4S_7. In contrast, annealing ML VS_2 in a S atmosphere forms V_5S_8, where V atoms have self-intercalated between the VS_2 layers in a 2×2 pattern. Surprisingly, we find that V_5S_8 has a layer-dependent CDW at low temperature, with bilayer V_5S_8 exhibiting a $\sqrt{3} \times \sqrt{3}$ CDW, while the trilayer hosts a striped CDW phase akin to that of ML VS_2.

O 56.9 Wed 17:00 GER 37

Nucleation stage for the oriented growth of tantalum sulfide monolayers on Au(111) — •Thais Chagas[1], Kai Mehlich[1], Abdus Samad[2], Catherine Grover[1], Daniela Dombrowski[1,3], Jiaqi Cai[1], Udo Schwingenschlögl[2], and Carsten Busse[1] — [1]Department Physik, Universität Siegen, Siegen, Germany — [2]Physical Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia — [3]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany

We study the nucleation stage in the epitaxial growth of monolayer TaS_2 as a model system for monolayer transition metal sulfides. The growth was done under ultra-high vacuum conditions with Au(111) as a substrate on which the metal atoms are evaporated, and the sulfur is provided from a background of H_2S. Using scanning tunneling microscopy (STM), we find small trimers with a well-defined triangular shape that act as nuclei for the further growth of extended tantalum sulfide monolayers. We identify these trimers as TaS_3 using density functional theory (DFT). We propose that the unique orientation of the trimers is the cause of the well-defined orientation of a complete TaS_2 layer found under favorable growth conditions.

O 56.10 Wed 17:15 GER 37

Growth and structure of two-dimensional single-layer HfS_2 on Au(111) — •Monika Schied, Paolo Lacovig, and Silvano Lizzit — Elettra-Sincrotrone Trieste

HfS_2 is a promising 2D material for low-power semiconductor devices due to its predicted high electron mobility and low contact resistance for n-type carrier transport. For actual applications, layers with excellent structural and electronic properties are needed. However, films with the necessary quality are only available from exfoliation, which is neither scalable nor very reproducible and only few experimental studies on a single-layer (SL) of HfS_2 have been performed so far. In analogy to the growth of high-quality SL transition metal dichalcogenides (TMDCs) such as MoS_2 and WS_2 [1,2] we have epitaxially grown an ordered layer of HfS_2 on Au(111) by chemical vapour deposition (CVD). Monitoring the S 2p and Hf 4f core levels in real time by fast X-ray photoelectron spectroscopy (XPS) allows the fine-tuning of the relevant parameters – such as the dosing rate and temperature – during the growth. The characterization by X-ray photoelectron diffraction (XPD) and low-energy electron diffraction (LEED) gives insight into the crystal structure of the film grown in this way.

[1] Bana, H., et.al., 2D Mater. 5 035012 (2018)
[2] Bignardi, L. et.al., Phys. Rev. Mat. 3, 014003, (2019)

O 57: Focus Session: Semiconductor Surface Chemistry – from Reaction Mechanisms to Well-Ordered Interfaces II

Time: Wednesday 15:00–17:00 Location: GER 38

Topical Talk O 57.1 Wed 15:00 GER 38

Incorporation of arsenic into silicon (001) and germanium (001) for atomic-scale device fabrication. — •Steven R. Schofield — London Centre for Nanotechnology, University College London, 17-19 Gordon St, WC1H 0AH, United Kingdom

Atomic-scale electronic devices can be fabricated via the deterministic placement of individual donor atoms in semiconductors. The commonly-used technique involves the thermal decomposition of phosphine on the Si(001) surface and the patterning of a hydrogen resist layer for spatial control. However, it is now established that the desorption of phosphorus from the surface during the thermal incorporation anneal limits the scale-up of this method, e.g., for the fabrication of large numbers of qubits. In this talk, I will present exciting new work in our group demonstrating the excellent characteristics of arsine adsorption to both Si(001) and Ge(001) for the creation of atomic-scale devices. I will present combined scanning tunnelling microscopy and density functional theory work demonstrating that arsenic incorporates into the Ge(001) surface at room temperature when exposed to arsine, thus eliminating the need for the thermal anneal that is so problematic for phosphine on Si(001). Furthermore, I will present soft x-ray angle-resolved photoelectron spectroscopy (SX-ARPES) measurements of delta-doped layers in silicon that demonstrate higher confinement for arsenic layers compared to phosphorus layers. Our new results offer exciting opportunities for the fabrication of donor-based devices and their scale-up to the large numbers of qubits required for the fabrication of technological quantum devices.

O 57.2 Wed 15:30 GER 38

Controlling tip-induced reaction products of surface-adsorbed organic species on Si(001) — •Alexa Adamkiewicz[1], Tamam Bohamud[1,2], Marcel Reutzel[1], Gerson Mette[1], Ulrich Höfer[1], and Michael Dürr[1,2] — [1]Department of Physics, Philipps University Marburg, Germany — [2]Institute of Applied Physics, Justus Liebig University Giessen, Germany

Tip-induced electronic excitation via STM can give access to alternative reaction channels beyond thermal activation. We showed for the cleavage of tetrahydrofuran (THF) on Si(001) that excitation by the tunneling electrons leads to new final products, which can be selectively addressed by the type of excitation [1]. Here, we present the influence of the detailed configuration of the organic adsorbates on tip-induced ether cleavage. Due to the linear molecular structure of diethyl ether (Et_2O), the adsorbates undergo fragmentation when cleaved, thus leading to a higher degree of freedom compared to the ring-shaped THF. The final products differ significantly for both species. Furthermore, we show that upon high voltage scans, covalently bound Et_2O fragments can be further reacted into more complex configurations which are thermally not accessible [2].

[1] Mette *et al.*, Angew. Chem. Int. Edit. **58**, 3417 (2019).

[2] Adamkiewicz *et al.*, J. Phys.: Condens. Matter **33**, 344004 (2021).

Topical Talk O 57.3 Wed 15:45 GER 38

Semiconductor surface chemistry towards hybrid interfaces with ab initio approaches — •Ralf Tonner-Zech — Universität Leipzig, Leipzig, Germany

Exploiting concepts from molecular chemistry helps to improve our understanding of organic molecules reacting with semiconductor surfaces like silicon or germanium. Electronic structure analysis reveals concepts like Pauli repulsion or nucleophilic substitution reactions. Starting from this, hybrid interfaces can step by step be designed and analysed. The talk will focus on the associated challenges for theory encompassing model building, accuracy, adsorption kinetics and conceptual understanding. Finally, interface design from theory will be outlined.

[1] Pecher, Tonner, WIREs Comput. Mol. Sci. 2019, 9, e1401. [2] Luy, Molla, Pecher, Tonner, J. Comput. Chem. 2021, 42, 827. [3] Glaser, Meinecke, Freund, Langer, Luy, Tonner, Koert, Dürr, Chem.–Eur. J. 2021, 27, 8082.

O 57.4 Wed 16:15 GER 38

Oxygen vacancy occupancy influences oxygen evolution on $BiVO_4$ — •Nicklas Österbacka, Hassan Ouhbi, and Julia Wiktor — Chalmers University of Technology, Gothenburg, Sweden

Bismuth vanadate, $BiVO_4$, is one of the best semiconductor photoanode materials for photoelectrochemical water splitting. Oxygen vacancies are abundant in the material and greatly affect its photoelectrochemical properties. If present at the surface, these defects could additionally directly influence the oxygen evolution reaction. The electronic occupancy of the defect states may also play a role, but are seldom considered in mechanistic studies.

In this work, we use hybrid density functional theory to show that the surface oxygen vacancy in bismuth vanadate is most stable in its fully ionized state. We investigate how this affects the mechanics of the oxygen evolution reaction and compare the pathway with those involving the unionized surface vacancy and the defect-free surface. To quantify whether or not vacancy ionization is beneficial, the thermodynamic overpotentials required to drive the reaction are also computed and compared.

O 57.5 Wed 16:30 GER 38

Adsorption and photocatalytic inactivation of SARS-CoV-2 and virus like particles on the surface of anatase TiO2(101) — •Mona Kohantorabi[1], Michael Wagstaffe[1], Marcus Creutzburg[1], Esko Erick Beck[1], Johannes Roessler[2], Reinhard Zeidler[2], Alexander Herrmann[3], Martin Feuerherd[3], Gregor Ebert[3], Gabriela Guédez[4], Christian Löw[4], Roland Thuenauer[4], Thomas F. Keller[1,5], Benedikt Sochor[6], Matthias Schwartzkopf[6], Andrei Chumakov[6], Stephan V. Roth[6], Ulrike Protzer[3], Wolfgang Hammerschmidt[2], Andreas Stierle[1,5], and Heshmat Noei[1] — [1]Centre for X-ray and Nano Science, DESY — [2]Helmholtz Zentrum München — [3]Technical University of Munich — [4]Centre for Structural Systems Biology, DESY — [5]Department of Physics, University of Hamburg — [6]Deutsches Elektronen-Synchrotron

In this contribution, adsorption of SARS-CoV-2 and SARS-CoV-2 like particles (VLPs) were investigated on the surface of the model photocatalyst TiO2(101). The samples were analyzed by grazing-incidence small-angle X-ray scattering (GISAXS), atomic force microscopy (AFM), transmission electron microscopy and X-ray photoelectron spectroscopy to obtain insight into the interaction of the SARS-CoV-2 and VLPs with the surface of TiO2(101). Furthermore, the UV induced photo inactivation of adsorbed species was investigated. AFM and GISAXS results on the UV-treated sample suggested that adsorbed viral particles undergo damage and photocatalytic oxidation on the surface of TiO2 which can affect the structural proteins.

O 57.6 Wed 16:45 GER 38

Ab initio description of surface restructuring and phase boundaries under realistic conditions — •Yuanyuan Zhou[1,3], Chunye Zhu[1,2], Matthias Scheffler[1], and Luca M Ghiringhelli[1] — [1]The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin — [2]School of Advanced Manufacturing, Guangdong University of Technology, Jieyang 515200, China — [3]Department of Physics, Technical University of Denmark, Kongens Lyngby, 2800, Denmark

A reliable description of surfaces equilibria in a reactive gas is a prerequisite for understanding mechanism of heterogeneous catalysis. However, studying phase equilibria at *ab initio* level, is a formidable challenge, especially for systems with sluggish barriers. In this work [Zhou *et al.* Phys. Rev. Lett. 128, 246101(2022)], we introduce a fully *ab initio* approach to determine temperature-pressure ($T-p$) surface phase diagram and to evaluate phase equilibria of surfaces in a gas phase. For this purpose, our replica-exchange grand-canonical (REGC) method [Zhou *et al.* Phys. Rev. B. 100, 174106(2019)], is extended by evaluating the heat capacity, $C_v(T,p)$, as function of T and p, thus locating phase boundaries where $C_v(T,p)$ shows ridges. The approach is demonstrated by addressing open questions for the Si(100) surface in a H_2 gas phase. 25 distinct stable surface phases are identified, most of which have not been observed experimentally, so far. The results also show that Si-Si-bonds forming/breaking is the driving force behind the experimentally 3×1 and 2×1 phase transition.

O 58: Plasmonics and Nanooptics II: Light-Matter Interaction and Spectroscopy I

Time: Wednesday 15:00–17:30 Location: WIL A317

O 58.1 Wed 15:00 WIL A317

Simultaneous Strong Coupling of the H- and J-Bands of Molecular Aggregates in Microcavities — •Roland Schäfer[1], Lukas Böhner[1], Manuela Schiek[2,3], Klaus Meerholz[1], and Klas Lindfors[1] — [1]Department für Chemie, Universität zu Köln, 50939 Köln, Germany — [2]LIOS & ZONA, Johannes Kepler Universität, 4040 Linz, Austria — [3]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany

We simultaneously strongly couple the H- and J-bands of aggregates of a merocyanine dye (HB238 [1]) to cavity photons. This is achieved by tuning the $3\lambda/2$- and 1λ mode of a planar microcavity to the spectral positions of the H- and J-bands, respectively. Strong coupling behavior is confirmed via the observation of Rabi-splitting of both bands in angle-resolved reflectivity spectra.

Due to the orientation of the aggregates J-polaritons can be observed with s- and p-polarized light, while the H-polaritons can only be accessed with p-polarized light and a non-normal angle of incidence. Therefore, our system supports two or four polaritons, depending on the polarization, making it an interesting platform to study strong light-matter coupling.

[1] Bürckstümmer, H., et. al., *Angew. Chem. Int. Ed.* **2011**, 50: 11628-11632.

Acknowledgment: This project is funded with support from the RTG-2591 "TIDE - Template-designed Organic Electronics" (Deutsche Forschungsgemeinschaft).

O 58.2 Wed 15:15 WIL A317

Two-Dimensional Electronic Spectroscopy of Strong Exciton-Surface Plasmon Polariton Coupling — •Daniel Timmer[1], Moritz Gittinger[1], Thomas Quenzel[1], Sven Stephan[1], Jennifer Zablocki[2], Arne Lützen[2], Jin-Hui Zhong[1], Martin Silies[1], Antonietta De Sio[1], and Christoph Lienau[1] — [1]University of Oldenburg, Germany — [2]University of Bonn, Germany

The creation of hybrid light-matter systems due to strong coupling is of major current interest for material science. Of special interest are dipolar interactions between molecular excitons (X) and plasmonic resonators, such as surface plasmon polaritons (SPP). Sufficiently strong coupling to vacuum field fluctuations allows for the coherent flow of energy between X and SPP, i.e. Rabi oscillations, forming new hybridized upper (UP) and lower (LP) polariton states [1]. We explore these strong coupling phenomena and especially their dynamics using two-dimensional electronic spectroscopy (2DES). Here, strong coupling predicts notorious "oscillating cross-peaks" between diagonal UP and LP peaks in a 2DES map. We investigate the polariton dynamics of a prototypical system for X-SPP coupling, a J-aggregate coated periodic gold slit array. In our measurements, the strongly coupled system indeed shows these hallmarks: Rabi oscillations of 2DES cross-peaks. Surprisingly, however, spatial modulations of the plasmon field seem to result in both strongly and weakly coupled excitons, which can then undergo coherent population transfer via the SPP. This conclusion is further supported by FDTD and Frenkel exciton model simulations. [1]: Vasa, Parinda, et al., Nat. Photon 7.2, 128-132 (2013).

Topical Talk O 58.3 Wed 15:30 WIL A317

Phase-locked photon-electron interaction without a laser — •Nahid Talebi — Institute for Experimental and Applied Physics, Kiel University, 24107 Kiel, Germany

Ultrafast electron-photon spectroscopy in electron microscopes commonly requires ultrafast laser setups. Photoemission from an engineered electron source is used to generate pulsed electrons, interacting with a sample that is excited by the ultrafast laser pulse at a specified time delay. Thus, developing an ultrafast electron microscope demands the exploitation of extrinsic laser excitations and complex synchronization schemes. Here, we present an inverse approach based on cathodoluminescence spectroscopy to introduce internal radiation sources in an electron microscope. Our method is based on a sequential interaction of the electron beam with an electron-driven photon source (EDPHS) and the investigated sample. An electron-driven photon source in an electron microscope generates phase-locked photons that are mutually coherent with the near-field distribution of the swift electron. Due to their different velocities, one can readily change the delay between the photons and electrons arriving at the sample by changing the distance between the EDPHS and the sample. We demonstrate the mutual coherence between the radiations from the EDPHS and the sample by performing interferometry with a combined system of an EDPHS and a WSe_2 flake. We assert the mutual frequency and momentum-dependent correlation of the EDPHS and sample radiation, and determine experimentally the degree of mutual coherence of up to 27%.

O 58.4 Wed 16:00 WIL A317

Layer-resolved resonance intensity of evanescent polariton modes — Nikolai C. Passler[1], Giulia Carini[1], Dmitry N. Chigrin[2,3], and •Alexander Paarmann[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]DWI - Leibniz-Institut für Interaktive Materialien, Aachen — [3]Institute of Physics (1A), RWTH Aachen University, Aachen

Most nanophotonic approaches rely on polaritons to confine light to the nanoscale. In particular heterostructures of strongly anisotropic polar crystals have been of key interest recently, where the twist angles between different anisotropic layers key be leveraged to create and control exotic polaritonic states [1]. To guide the designs of such multiparameter systems, low-cost simulation tools are invaluable. Common approaches like employing the reflection coefficient under evanescent excitation enable analysis of the polariton resonances without the need to specify the exact experimental arrangement, but lack layer-specific information. Here [2], we introduce a formalism based on a 4x4 transfer matrix algorithm [3] and energy flow analysis using the Poynting vector [4], that provides full depth-resolved information even for evanescent wave excitation. We illustrate the power of the approach by analysing a state-of-the-art example of twisted bilayer molybdenum trioxide [1].

[1] G. Hu, et al., Nature 582, 209 (2020).
[2] N.C. Passler, et al., arXiv preprint, arXiv:2209.00877 (2022).
[3] N.C. Passler & A. Paarmann, JOSA B 34, 2128 (2017).
[4] N.C. Passler, et al., PRB 101, 165425 (2020).

O 58.5 Wed 16:15 WIL A317

Observation of multi-quantum phenomena in molecular films strongly coupled to surface plasmons using ultrafast laser spectroscopy — •Simon Büttner[1], Matthias Hensen[1], Katja Mayershofer[1], Maximilian Rödel[2], Jens Pflaum[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Experimental Physics VI, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Multi-quantum phenomena such as exciton–exciton annihilation can be used to study exciton diffusion [1], which is a key process in optoelectronic devices like solar cells. Recently, our group has developed a method to isolate different multi-quantum signals using transient absorption (TA) spectroscopy. This novel method makes it possible to filter out the interaction of a distinct number of quasiparticles and their time evolution. Here, we use this method together with a new ultrafast laser setup that allows us to shape and detect femtosecond laser pulses at a repetition rate of 100 kHz. As a model system we investigate a thin Zinc phthalocyanine (ZnPc) film on a surface-plasmon-supporting gold substrate. Strong coupling between ZnPc excitons and surface plasmons leads to the formation of plexcitons [2], and thus to a delocalization of charge carriers, which is of particular interest for increasing charge carrier mobilities. In this work we focus on the influence of the strong coupling on the quasiparticle diffusion.

[1] P. Malý et al., *Chem. Sci.* 11, 456 (2020)
[2] M. Rödel et al., *J. Phys. Chem. C* 126, 4163-4171 (2022)

O 58.6 Wed 16:30 WIL A317

Resonant imaging of infrared light confinement using phonon polaritons in sub-diffractional 4H-SiC nanostructures — •Richarda Niemann[1], Sören Wasserroth[1], Guanyu Lu[2], Christopher R. Gubbin[3], Martin Wolf[1], Simone de Liberato[3], Joshua D. Caldwell[2], and Alexander Paarmann[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Vanderbilt University, Nashville, USA — [3]University of Southampton, UK

Confinement of light to deeply sub-wavelength scales can be achieved using polaritons spatially confined to sub-diffractional nanostructures.

Next to well-established plasmon polariton approaches, phonon polaritons supported in nanostructures made from polar dielectric crystals are a promising tool for the infrared spectral range [1].

Here, we study localized phonon polariton resonances in sub-diffractional 4H-SiC nanostructures using infrared super-resolution sum-frequency generation (SFG) microscopy [2], employing our institute's infrared free-electron laser [3]. With this technique we achieve high sensitivity to optical field enhancement associated with the spatial confinement of light. Simultaneously it is providing sub-diffractional imaging resolution, naturally enabling to study polaritons on their intrinsic length scales.

[1] Gubbin et al., Journal of Appl. Phys. 131, 030901 (2022)
[2] Niemann et al., Appl. Phys. Lett. 120, 131102 (2022)
[3] Schöllkopf et al., Proc. SPIE 9512, 95121L (2015)

O 58.7 Wed 16:45 WIL A317

Nano-scale Plasmonic Su-Schrieffer-Heeger Chains — •Benedikt Schurr[1,4], Philipp Grimm[1], Tobias Helbig[2], Tobias Hofmann[2], Lukas Wehmeier[3], Felix G. Kaps[3], Thorsten Feichtner[1,4], Monika Emmerling[1], Susanne C. Kehr[3], Lukas Eng[3,4], Ronny Thomale[2,4], and Bert Hecht[1,4] — [1]NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — [4]Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

The tight-binding Su-Schrieffer-Heeger (SSH) model describes 1D periodic chains of resonators with alternating coupling strengths. For certain configurations, topologically protected collective states occur at the edges. Here, we propose a plasmonic chain SSH-system with alternating few-nanometer gaps, fabricated from mono-crystalline Au-microplatelets by means of He-ion beam milling. Full FDTD simulations show the occurrence of edge modes for such geometries in real space. The frequency at which edge states occur can be fully controlled via particle size and the next-neighbour coupling via the gaps. Scattering scanning near-field optical microscopy (sSNOM) experiments provide first evidence for the presence of topologically protected edge states.

O 58.8 Wed 17:00 WIL A317

Directional leaky polaritons in anisotropic crystals — Xiang Ni[1], •Giulia Carini[2], Weiliang Ma[3], Enrico M. Renzi[1], Emanuele Galiffi[1], Sören T. Wasserroth[2], Martin Wolf[2], Peining Li[3], Alexander Paarmann[2], and Andrea Alù[1] — [1]CUNY, New York, USA — [2]FHI, Berlin, Germany — [3]HUST, Wuhan, China

For quite a few years now, natural hyperbolic materials have been attracting significant attention due to their ability of engaging strong interactions between light and their IR active phonon resonances. The hybridized light-matter quasiparticles arising in their bulk, known as hyperbolic phonon polaritons, display large momenta and highly directional propagation stemming from their open topology.

In our contribution, we demonstrate a new class of directional polaritons supported in the lower reststrahlen band of calcite, that feature lenticular isofrequency contours. These novel polaritons, dubbed Leaky Polaritons (LPs), arise in the type-I in-plane hyperbolic region as hybridized states between extraordinary surface-bound and ordinary propagating bulk modes. Despite their closed topology, they support highly directional, long-range, sub-diffractive propagation at the interface. Their dispersion curve also crosses the free-space light cone, providing radiative far-field coupling to both sides of the interface.

To observe the features of LPs experimentally, we employed polariton spectroscopy, far-field probing and near-field imaging, revealing their lenticular dispersion curve, their high directionality, their long lifetime and real-space propagation.

O 58.9 Wed 17:15 WIL A317

Anticrossing of a plasmonic nanoresonator mode and a single quantum dot at room temperature — •Daniel Friedrich[1], Jin Qin[1], Benedikt Schurr[1], Tommaso Tufarelli[2], Heiko Gross[1], and Bert Hecht[1] — [1]NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany — [2]School of Mathematical Sciences and Centre for the Mathematics andTheoretical Physics of Quantum Non-Equilibrium Systems, Universityof Nottingham, United Kingdom

At ambient conditions strong coupling (SC) is achieved due to the extremely small mode volume of plasmonic nanoresonators and the broadband spectral overlap between emitter and nanocavity. This results in ultrafast energy transfer which overcomes dephasing. Normal mode splittings in luminescence spectra of single quantum systems coupled to plasmonic nanoresonators have been reported and exploited to estimate the light-matter coupling strength g. However, there is only sketchy evidence for the hallmark of single-emitter strong coupling, the anticrossing of emitter and cavity resonances. Here, we exploit the light-induced oxygen-dependent blue-shift of individual CdSe/ZnS semiconductor quantum dots to tune their transition energy across the weakly radiative resonance of a scanning plasmonic slit resonator. The observed anticrossing in photoluminescence spectra recorded as a function of time provide clear proof of SC as well as a solid measure for the single-emitter coupling strength consistent with classical field simulations and a quantum model including dissipation.

O 59: Electronic Structure of Surfaces I

Time: Wednesday 15:00–17:45 Location: REC C 213

Topical Talk O 59.1 Wed 15:00 REC C 213

Interplay of Inversion Symmetry Breaking and Spin-Orbit Coupling — •Maximilian Ünzelmann — Experimentelle Physik 7, Universität Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat

Inversion symmetry breaking (ISB) in crystalline solids provides an essential way of modifying electronic structures. For example, in combination with spin-orbit coupling (SOC), ISB allows for a lifting of spin degeneracy without the need for magnetism. Moreover, it is a source of Berry curvature, which is of fundamental importance in topological quantum matter. In this talk, two scenarios will be discussed, in which the interplay of ISB with SOC plays an important role: (i) At surfaces or interfaces, where inversion symmetry is inherently broken and the Rashba effect [1] enforces a locking of the electrons spin perpendicular to its momentum and (ii) in Weyl semimetals whose three-dimensional crystal structure has no inversion center, leading to the formation of Berry curvature monopoles, i.e., quantized topological charges [2].

As will be highlighted in this presentation, we find that ISB-induced unquenching of the so-called (atomic) orbital angular momentum (OAM) in the Bloch wave functions constitutes a key mechanism underlying the physics of both the Rashba effect and Weyl semimetals. Angle-resolved photoemission with variable light polarization provides detailed experimental access to the respective momentum-space orbital textures.

[1] M. Ünzelmann et al., Phys. Rev. Lett. **124**, 176401 (2020)
[2] M. Ünzelmann et al., Nat. Commun. **12**, 3650 (2021)

O 59.2 Wed 15:30 REC C 213

Unoccupied surface electronic structure of Re(0001) — •Fabian Schöttke, Sven Schemmelmann, Peter Krüger, and Markus Donath — Westfälische-Wilhelms-Universität Münster, Germany

The influence of spin-orbit interaction on the unoccupied electronic structure of the Re(0001) surface is investigated by spin- and angle-resolved inverse photoemission and density-functional theory calculations. In the two high-symmetry azimuths $\overline{\Gamma}\,\overline{K}$ and $\overline{\Gamma}\,\overline{M}$, we identify transitions into d-derived bulk states as well as different types of surface states. The Rashba-type spin-split hole pocket around $\overline{\Gamma}$ finds continuation in empty spin-split surface states for higher $\mathbf{k}_{\parallel}$, thereby forming W-shaped states whose lower parts are partially occupied.

Schöttke *et al.*, Phys. Rev. B **105**, 155419 (2022).

O 59.3 Wed 15:45 REC C 213

Establishing fundamentals of ARPES spin textures with the model material 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

A novel quantum material $PtTe_2$ is used to establish the connection between spin textures of angle-resolved photoemission spectroscopy (ARPES) and initial state spin textures. The crystal structure of 1T-$PtTe_2$ is trigonal, belongs to the space group 164 ($P\bar{3}m1$), that contains mirror planes and inversion symmetry. Since bulk 1T-$PtTe_2$ is both inversion-symmetric and non-magnetic, no bulk spin-polarized bands are allowed due to the Kramers degeneracy. At the surface, a non-zero spin polarization is expected due to the broken inversion symmetry, however, it must obey the mirror and time-reversal symmetries.We measured the dependence of the spin-polarization on the symmetries of the ARPES setup. This is performed in two geometries, with the reaction plane parallel to $\bar{K}$-$\bar{\Gamma}$-$\bar{K}$ and $\bar{M}$-$\bar{\Gamma}$-$\bar{M}$ reciprocal directions, i.e. either along or orthogonal to the crystal mirror plane. The measured spin texture is symmetric when the reaction plane is parallel to $\bar{K}$-$\bar{\Gamma}$-$\bar{K}$. However, we see asymmetries in the spin texture when the reaction plane is parallel to $\bar{M}$-$\bar{\Gamma}$-$\bar{M}$. For surface states, the asymmetries are due to the geometry-induced spin filtering in ARPES [1]. For bulk states, the effect might be additionally related to the asymmetric initial state dispersions. [1] T. Heider et al., arXiv:2210.10870 (2022)

O 59.4 Wed 16:00 REC C 213

Surface electronic structure of Re(0001): A spin-resolved photoemission study — •Marcel Holtmann[1], Peter Krüger[2], Koji Miyamoto[3], Taichi Okuda[3], Shiv Kumar[3], Kenya Shimada[3], and Markus Donath[1] — [1]Physikalisches Institut, WWU Münster, Germany — [2]Institut für Festkörpertheorie, WWU Münster, Germany — [3]HiSOR, Hiroshima University, Japan

The surface electronic structure of Re(0001) has been investigated in a combined experimental and theoretical study. (Spin- and) angle-resolved photoemission was employed to unravel the spin-dependent $E(\mathbf{k}_{\|})$ dispersion along the $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{K}}$ directions. The results are compared with band structures from density-functional theory. Moreover, transitions into final states have been considered by inclusion of the corresponding matrix elements. A spin-orbit-induced mixing of Shockley- and Tamm-type surface states around $\overline{\Gamma}$ and close to E_F was reported recently [1]. Here, we extend the analysis to a wider $E(\mathbf{k}_{\|})$ range showcasing a multitude of electronic states along the $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{K}}$ directions. In particular, Rashba-type spin splittings are observed around the high-symmetry $\overline{\Gamma}$ and $\overline{\mathrm{M}}$ points. At variance with theoretical predictions [2], which describe a perfect hcp(0001) surface, we do not find any out-of-plane spin polarization. This is caused by monoatomic steps of a real Re(0001) surface with alternating terminations, which lead on average to an effective sixfold surface symmetry and vanishing net out-of-plane spin polarization.

[1] M. Holtmann *et al.*, Phys. Rev. B **105**, L241412 (2022)

[2] A. Urru and A. Dal Corso, Surf. Sci. **686**, 22 (2019)

O 59.5 Wed 16:15 REC C 213

Spectroscopic evidence for a new type of surface resonance at noble-metal surfaces — •Tobias Eul[1], Jürgen Braun[2], Benjamin Stadtmüller[1,3], Hubert Ebert[2], and Martin Aeschlimann[1] — [1]Technische Universität Kaiserslautern and Research Center OPTIMAS, 67663 Kaiserslautern, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany — [3]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

We investigated the surface and bulk properties of the pristine (110) surface of silver using threshold photoemission by excitation with light of 5.9 eV. Using a momentum microscope, we identified two distinct transitions along the $\overline{\Gamma Y}$-direction of the crystal. The first one is a so far unknown surface resonance of the (110) noble-metal surface, exhibiting an exceptionally large bulk character that has so far been elusive in surface sensitive experiments. The second one stems from the well-known bulklike Mahan cone oriented along the ΓL-direction inside the crystal but projected onto the (110)-surface cut. The existence of the new state is confirmed by photocurrent calculations, and its character is analyzed.

O 59.6 Wed 16:30 REC C 213

One monolayer of Tl on Ag(111): Hybridization of image-potential states with Tl states — •Sven Schemmelmann[1], Patrick Härtl[2], Peter Krüger[3], Matthias Bode[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster — [2]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg — [3]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, Münster

For one atomic layer of Tl on Ag(111) a moiré superstructure is observed. The unoccupied electronic structure of this superstructure is investigated by spin- and angle-resolved inverse photoemission. The experimental results are interpreted on the basis of DFT calculations. We observe several Tl-induced surface states and an image-potential state mainly located several Å in front of the surface. Surprisingly, we find a hybridization of this image state with a downward dispersing Tl band. This leads to spin-dependent spectral intensities that vary rapidly close to the hybridization point. The calculations show an expeditious change of the charge density from a resonant image-potential state towards a Tl-induced surface state in dependence of $\mathbf{k}_{\|}$.

O 59.7 Wed 16:45 REC C 213

Bulk and surface electronic structure of tunnel barrier Nb_3Br_8 in the field-free Josephson diode — •Mihir Date[1,2], Jonas.A. Krieger[1], Emily.C. McFarlane[1], Vicky Hasse[3], Claudia Felser[3], Stuart.S.P Parkin[1], Matthew Watson[2], and Niels.B.M Schröter[1] — [1]MPI-Halle, Weinberg 2, 06120 Halle (Saale), Germany — [2]Diamond Light Source Ltd. Didcot, OX11 0DE, United Kingdom — [3]MPI-CPfS, Nöthnitzer Straße 40, 01187 Dresden, Germany

In this work, we report the bulk and surface electronic structure of Nb_3Br_8 probed using angle resolved photoemission spectroscopy (ARPES). Nb_3Br_8 is predicted to host trivial metallic surface states (obstructed surface states (OSS)) when cleaved between specific layers [1]. Although our in-plane electronic structure is consistent with the calculated orbital resolved bandstructure, we do not observe any signatures of the OSS. Nevertheless, the doubling of periodicity of the ARPES signal along the out-of-plane momentum direction, as compared to the Brillouin zone dimension, hints towards dimerization between alternate layers through the OSS. We discuss our results in connection with the recent discovery of the field-free Josephson diode effect in the $NbSe_2/Nb_3Br_8/NbSe_2$ heterostructures [2].

[1] Xu, Y. et al. arXiv:2106.10276 (2021).

[2]. Wu, H. et al. Nature 604 (2022).

O 59.8 Wed 17:00 REC C 213

Termination dependent many-body interactions of the surface states of $PdCoO_2$ revealed by ARPES-based microscopy — •Gesa-Roxanne Siemann[1], Edgar Abarca Morales[1,2], Philip A. E. Murgatroyd[1], Tommaso Antonelli[1], Seunghyun Khim[2], Matthew Watson[3], Cephise Cacho[3], Andrew P. Mackenzie[1,2], and Phil D. C. King[1] — [1]University of St Andrews, UK — [2]MPI for Chemical Physics of Solids, Dresden, Germany — [3]Diamond Light Source, UK

The layered ABO_2 structure of the delafossite oxides yields markedly different electronic structures at their A- and BO_2-terminated surfaces which are either electron- (A-termination) or hole-doped (BO_2-termination) with respect to the bulk[1]. A prominent example is $PdCoO_2$ where a giant Rashba effect can be observed on the CoO_2 terminated surface[2], while the Pd terminated surface hosts ferromagnetic states which are absent in the bulk[3,4]. However, the study of these states has often been hampered by the size of domains of each distinct surface termination. Here we show how these problems can be circumvented using micro-ARPES performed in a spatially-resolved mode. Our measurements further reveal strong signatures of self-energy modulations on both surfaces due to coupling to bosonic modes, making them the ideal playground to study varying coupling mechanisms and their tunability in the same sample. [1]A. P. Mackenzie, Rep. Prog. Phys. 80, 032501 (2017), [2]V. Sunko et al., Nature 549, 492-496 (2017), [3]F. Mazzola et al., PNAS 115(51)12956-12960 (2018), [4]F. Mazzola et al., npj Quantum Materials 7, 20 (2022)

O 59.9 Wed 17:15 REC C 213

The Meservey-Tedrow-Fulde vortex in epitaxial aluminum near the monolayer limit — •Werner M.J. van Weerdenburg[1], Anand Kamlapure[1], Eirik Fyhn Holm[2], Niels P.E. van Mullekom[1], Xiaochun Huang[1], Manuel Steinbrecher[1], Peter Krogstrup[3], Jacob Linder[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University Nijmegen, the Netherlands — [2]Center for Quantum Spintronics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway — [3]NNF Quantum Computing Programme, Niels Bohr Institute, University of Copenhagen, Denmark

The critical magnetic field of 2D superconductors is greatly enhanced for fields parallel to the 2D plane. In the case of aluminum, this gives rise to a spin-splitting of the coherence peaks, referred to as the Meservey-Tedrow-Fulde (MTF) effect. In the MTF regime, it has been proposed that unconventional odd-frequency (ω_o) spin-triplet pairing is promoted [1], but their presence is experimentally hard to detect. Here, we study vortices in thin epitaxial Al films on Si(111) in the MTF regime by applying a vector magnetic field with a large in-plane component, and find experimental evidence of odd-frequency pairing [2]. Strikingly, we find that the shape of the vortex structure is strongly modified and exhibits a gapless region. Numerical simulations confirm a connection between this vortex shape and the presence of ω_o pairing, highlighted by a paramagnetic Meissner effect.

[1] J. Linder & J. Robinson, Scientific Reports **5**, 15483 (2015)

[2] W. van Weerdenburg et al., arXiv:2210.10645 (2022)

O 59.10 Wed 17:30 REC C 213

Exploring polaron stability and defect structures in $\mathbf{Li_4Ti_5O_{12}}$ (LTO): A combined theoretical and experimental approach — •Yu-Te Chan[1], Matthias Kick[2], Cristina Grosu[2], Christoph Scheurer[1], and Harald Oberhofer[3] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Massachusetts Institute of Technology, Cambridge, USA — [3]University of Bayreuth, Bayreuth, Germany

Spinel $Li_4Ti_5O_{12}$ (LTO) is a promising anode material for next-generation all-solid-state Li-ion batteries (ASSB) due to its "zero strain" charge/discharge behavior. Pristine LTO suffers from poor ionic and electronic conductivity. Oxygen vacancies, produced by tailored sintering protocols, yield a performant, blue LTO material. Vacancy induced polarons have been proposed as one of the origins of increased electronic conductivity. However, detailed knowledge about polaron stability, distribution, and dynamics in LTO bulk and surface have been lacking. By performing *Hubbard corrected density functional theory* (DFT+U) calculations we are able to show that in fact polaron formation and a possible polaron hopping mechanism can not only play a significant role in enhancing electronic conductivity but boost Li^+ diffusion nearby, in line with the experimentally observed improved conductivities.[1,2] In combination with positron lifetime spectroscopy data and machine learning models, we arrive at a rather complete picture of the bulk vs. surface defect chemistry in LTO particles and the resulting mixed ionic electronic conductivity. [1] M. Kick et al., J. Phys. Chem. Lett. 11 (2020), 2535 [2] M. Kick et al., ACS Appl. Energy Mater 4 (2021), 8583

O 60: Solid-Liquid Interfaces I: Structure and Spectroscopy

Time: Wednesday 15:00–18:00 Location: TRE Phy

O 60.1 Wed 15:00 TRE Phy

Investigation of the water structure at the (001) and (010) orthoclase surfaces with three-dimensional atomic force microscopy — •Franziska Sabath, Ralf Bechstein, and Angelika Kühnle — Physical Chemistry I, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld

Feldspars are the most abundant minerals in the Earth's crust and belong to the most effective group of mineral ice nucleating particles (INP) in the atmosphere. In the crystal structure, potassium, sodium or calcium, among others, are incorporated as counterions in varying ratios. Potassium-rich feldspars are more effective INPs than the other feldspars. A representative of a potassium-rich feldspar is orthoclase. Unlike other INPs, such as silver iodide, the surfaces of feldspar do not have an ice-like structure. Therefore, it is interesting to know what other factors, such as hydroxyl groups on the surfaces or defect sites, are responsible for the high ice nucleating efficiency of K-feldspars. In particular, the water structure at the interface of K-feldspars is of interest. Here, we show the three-dimensional water structure at the two natural cleavage planes of orthoclase, the (001) and the (010) surfaces, using tree-dimensional atomic force microscopy (AFM).

O 60.2 Wed 15:15 TRE Phy

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

Self-assembly of supramolecular nanostructures at the solid-liquid interface has gained increasing academic interest in past recent years. Substrates can influence molecule-substrate interactions, which plays an important role in determining supramolecular nanostructures. In this study, we used scanning tunneling microscopy (STM) to investigate the self-assembly of two carboxylic acids at the nonanoic acid-solid interface. We performed the experiments on four substrates: HOPG, MoS2, Au(111), and graphene/Cu foil. We also measured the water contact angle of these four substrates to obtain some information on the molecule-substrate interaction. The STM measurements showed that, on HOPG and graphene/Cu foil, both carboxylic acids can form porous and close-packed structures, which depends on the bias voltage polarity during STM measurements. On MoS2, both carboxylic acids did not form stable self-assembled structures. On Au(111), both carboxylic acids only formed short range-ordered structures in very diluted solutions. The results reveal that the interplay between molecule-substrate, solvent-substrate and molecule-molecule interactions is important to the formation of supramolecular nanostructures at the solid-liquid interface.

O 60.3 Wed 15:30 TRE Phy

Hydrophobic pockets on the hydrophilic $\mathbf{In_2O_3}$(111) surface — Christian Ritterhoff[1], •Bernd Meyer[1], Ulrike Diebold[2], and Margareta Wagner[2] — [1]Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany — [2]Institute of Applied Physics, TU Wien, Austria

Clean oxide surfaces are generally hydrophilic. Water molecules anchor at undercoordinated surface cations that act as Lewis acid sites, and they are stabilized by H bonds to surface oxygens. However, for In_2O_3(111), DFT calculations predict a deviation from this general rule, which has been confirmed by TPD, XPS, STM and AFM experiments. In UHV, the first nine water molecules cover only a part of the unit cell. Within the H-bonded network three out of the nine water dissociate. Additional molecules pile up above the OH groups. The rest of the unit cell is unfavorable for adsorption and remains water-free, despite offering undercoordinated In and O sites. The first water layer thus shows ordering into nanoscopic 3D water clusters separated by hydrophobic pockets. Beyond UHV, our *ab initio* MD simulations of a liquid water layer demonstrate the robustness of the strongly hydrophobic behavior of this region in the unit cell.

[1] H. Chen, M.A. Blatnik, C.L. Ritterhoff, I. Sokolović, F. Mirabella, G. Franceschi, M. Riva, M. Schmid, J. Čechal, B. Meyer, U. Diebold, M. Wagner, ACS Nano, accepted, DOI: 10.1021/acsnano.2c09115

O 60.4 Wed 15:45 TRE Phy

Facet-dependent surface charge and hydration of SrTiO3 nanoparticles at variable pH — •Igor Siretanu, Su Shaoqiang, Bastian Mei, Dirk van den Ende, Guido Mul, and Frieder Mugele — Physics of Complex Fluids and Photocatalytic Synthesis Groups, MESA+ Institute, Faculty of Science and Technology, University of Twente, PO Box 217, 7500 AE Enschede, The Netherlands

Anisotropy of shape and surface properties determine the functionality of faceted nanoparticles in various contexts including facet selective colloidal self-assembly, biosensing, improved photo/electrocatalytic activity and ions uptake. The characteristic surface proprieties and function of solid-liquid interfaces of crystalline faceted nanoparticles are believed to be essential for their performance but remains poorly understood and difficult to characterize and quantify. We use dual scale Atomic Force Microscopy to measure electrostatic and hydration forces of faceted SrTiO3 nanoparticles in aqueous electrolyte at variable pH. We demonstrate (i) the ability to quantify strongly facet-dependent surface charges yielding isoelectric points of the dominant {100} and {110} facets that differ by as much as 2 pH units, ii) fluids composition controlled facet-dependent accumulation of oppositely charged (SiO2) particles, and iii) that atomic scale defects can be resolved but are in fact rare for the samples investigated. Atomically resolved images and facet-dependent hydration structure suggest a microscopic hydration and charge generation mechanism.

O 60.5 Wed 16:00 TRE Phy

Watching Redox Activation of Gold for Water Electrolysis live: An in-situ Experiment at Home — Christoph Griesser, Daniel Winkler, Toni Moser, Engelbert Portenkirchner, and •Julia Kunze-Liebhäuser — Institute of Physical Chemistry, University of Innsbruck, Innrain 52c, Innsbruck, 6020 Austria

A fundamental understanding of processes that take place at the solid/liquid interface is of utmost importance for a rational design of (electro-)catalysts, and key for advancing energy conversion and storage technologies. We could show with in-situ electrochemical near ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) that metallic Au, in alkaline media, reversibly oxidizes to Au$^+$ at potentials prior to and during the early oxygen evolution reaction (OER), while it reversibly oxidizes to Au^{3+} at potentials where the OER takes place at high rates. This has previously not been clearly demonstrated in-situ, so that the redox chemistry of Au in alkaline media remains a highly debated topic in the electrochemical community to date. We demonstrate the implementation of a simple, affordable and in-situ/operando- method to track dynamic processes taking place at the electrified solid/liquid interface, utilizing a lab-based NAP-XPS system with a conventional Al Kα X-ray source. The method has the potential to become a gamechanger in applied (electro-)catalysis research, which makes our contribution appealing for scientists following either fundamental or applied research interests.

O 60.6 Wed 16:15 TRE Phy

Structure and Reactivity of an Ionic Liquid on Cu(111) investigated by Scanning Probe Microscopy, Photoelectron Spectroscopy and Simulations — Rajan Adhikari[1], Stephen Massicot[1], Lukas Fromm[2], •Simon Jaekel[1], Timo Talwar[1], Afra Gezmis[1], Manuel Meusel[1], Andreas Bayer[1], Florian Maier[1], Andreas Görling[2], and Hans-Peter Steinrück[1] — [1]Chair of Physical Chemistry II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany — [2]Chair of Theoretical Chemistry, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

We studied the adsorption and reaction behaviour of the ionic liquid (IL) 1,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide ([C$_1$C$_1$Im][Tf$_2$N]) on Cu(111) in UHV. Our nc-AFM and STM results show that the IL transitions from an ordered structure observed after annealing at 200 K into a different ordered structure and disordered islands after extended annealing at 300 K. Complementary, ARXPS reveals that the IL initially adsorbs intact and that no IL desorption occurs until 300 K but that a significant fraction of the IL is converted to a new species. We correlate the remaining unshifted peaks to the ordered phases observed in AFM and the shifted peaks to decomposition products, which appear as disordered islands. From DFT, we obtain additional information on the structure of the ordered phases and the interaction of the IL with the substrate.

O 60.7 Wed 16:30 TRE Phy

Influence of Interfacial Water and Cations on the Oxidation of CO at the Platinum/Ionic Liquid Interface — •Björn Ratschmeier, Gina Ross, Andre Kemna, and Björn Braunschweig — University Münster, Institute of Physical Chemistry, Münster, Germany

CO oxidation is fundamental key for complete oxidation of small alcohols on Pt catalysts in fuel cells. So far, room-temperature ionic liquids (RTIL) have been used to modify the selectivity in electrocatalysis. In order to understand the mechanism of CO oxidation in RTIL we have investigated this reaction at the Pt(111)/1-butyl-3-methylimidazolium trifluorosulfonylimide [BMIM][NTf$_2$] electrode/electrolyte interface as a function of H$_2$O concentration and electrode potential using *in situ* sum-frequency generation (SFG) spectroscopy and infrared absorption spectroscopy (IRAS). Using SFG spectroscopy, we address the changes of CO molecules on Pt(111), while we monitor bulk electrolyte changes with IRAS using vibrational bands from H$_2$O, CO$_2$ and CO. The presence of water in [BMIM][NTf$_2$] shifts the CO onset potential by more than 200 mV with increased H$_2$O concentration from 0.01 to 1.5 M, which we relate to the incorporation and availability of water at the electrode/electrolyte interface. The nature of the RTIL cation has also a large effect on the surface excess of H$_2$O since RTILs which are prone to form closed-packed structures like [BMMIM][NTf$_2$] can block the incorporation of H$_2$O and lead to more sluggish CO oxidation with larger overpotentials and oxidation in a much broader potential.

O 60.8 Wed 16:45 TRE Phy

Resolving the structure of Cu(100) in iodine containing solutions — •Nicolas G. Hörmann, Nicolas Bergmann, Karsten Reuter, Beatriz Roldán Cuenya, Georg H. Simon, and Christopher S. Kley — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present results from our joint experimental and theoretical effort to identify the structure of iodine adlayers on Cu(100) in electrochemical environment – a first step towards understanding the origin of the influence of iodine on the electrocatalytic carbon dioxide reduction (CO2RR) on Cu. In particular, we resolve stable interface structures as a function of the potential by a detailed analysis of theoretical predictions from density functional theory calculations and in-situ EC-AFM measurements. These results are complemented by the comparison of experimental and theoretically simulated Cyclic Voltammograms [1,2], which provide additional information on electrosorption reactions and thereby the interface composition as a function of the potential.

[1] N.G. Hörmann et al., *J. Chem. Theory Comput.* **17**(3), 1782-1794 (2021). [2] N.G. Hörmann et al., *J. Phys. Condens. Matter.* **33**, 264004 (2021).

O 60.9 Wed 17:00 TRE Phy

Non-Random Island Nucleation in the Electrochemical Roughening on Pt(111) — •Marcel Rost[1], Leon Jacobse[2], and Marc Koper[3] — [1]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands — [2]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, D-22607 Hamburg, Germany — [3]Leiden Institute of Chemistry, Leiden University, Einsteinweg 55, 2333 CC Leiden, The Netherlands

Many chemical surface systems develop ordered nano-islands during repeated reaction and restoration. Platinum is used in electrochemical energy applications, like fuel cells and electrolysers, although it is scarce, expensive, and degrades.

During oxidation-reduction cycles, simulating device operation, nucleation and growth of nano-islands occurs that eventually enhances the dissolution. Preventing nucleation would be the most effective solution. However, little is known about the atomic details of the nucleation; a process almost impossible to observe.

Here, we analyze the nuclei-distance distribution mapping out the underlying atomic mechanism: a rarely observed, non-random nucleation takes place. Special, preferential nucleation sites that a priori do not exist, develop initially via a precursor and eventually form a semi-ordered Pt-oxide structure.

This precursor mechanism seems to be general, possibly explaining also the nano-island formation on other surfaces/reactions.

O 60.10 Wed 17:15 TRE Phy

Electrochemical re-structuring of the InP(100)-HCl interface monitored by operando reflection anisotropy spectroscopy — •Margot Guidat[1,2], Mario Löw[2], Daniel Lörch[1], Vibhav Yadav[1], Jongmin Kim[1,2], and Matthias M. May[1,2] — [1]Institute of Physical and Theoretical Chemistry, Universität Tübingen, Germany — [2]Institute of Theoretical Chemistry, Universität Ulm, Germany

A possible way to achieve a low-carbon energy system consists of hydrogen production by photoelectrochemical water splitting. Here, III-V semiconductors play an important role due to their high solar-to-hydrogen efficiencies. However, surface corrosion limits the overall performance of photoelectrochemical devices. Studies have reported that interface functionalization is a way to protect the surface. In this work, we monitor the potential-dependent restructuring of the electrochemical InP(100) interface in HCl by operando reflection anisotropy spectroscopy (RAS) [1]. We investigate the effect of electrolyte concentration on the ordering and stabilization of the surface film formed at cathodic potentials. Computational RAS qualitatively supports the formation of an InCl$_x$ layer. The latter is further investigated quantitatively with other characterization techniques. Fitting RA-transients measured under applied potentials with adsorption isotherm models gives insight into the lifetime of the involved processes and their adsorption energies. [1] Löw, M.; Guidat, M.; Kim, J.; May, M. M. RSC Adv. 2022, 12 (50), 32756-32764.

O 60.11 Wed 17:30 TRE Phy

A femtosecond resolved view of vibrationally assisted electron transfer across the metal/aqueous interface — •Zhipeng Huang, Manuel Bridger, Oscar Andres Naranjo-Montoya, Alexander Tarasevitch, Uwe Bovensiepen, Yujin Tong, and R. Kramer Campen — Faculty of Physics, University of Duisburg-Essen

Understanding heterogeneous charge transfer is crucial if we are to build the best electrolyzers, fuel cells and photoelectrochemical water splitting devices that chemistry allows. Since the elementary processes involved have characteristic timescales ranging from femto- to milliseconds, direct simulation of all relevant processes is not generally possible.

Here we demonstrate experimentally, using a novel two photon photovoltage approach, that for a prototypical system, a ferrocene terminate alkane thiol self-assembled monolayer (SAM) on gold in contact with aqueous electrolyte, charge transfer from the Au to the ferrocene can be induced by vibrational excitation of the ferrocene aromatic CH. Intriguingly the energy of the aromatic CH vibration, 0.38 eV, is a large fraction of the effective solvent interaction strength inferred for the ferrocene/ferrocenium system in prior electrochemical studies: 0.85 eV. Our results thus imply that, solvent may effect reduction/oxidation rates in electrocatalysis by coupling to a few, perhaps widely different in energy, vibrations. If shown to be generally true such a picture would suggest the necessity of moving beyond a single effective solvent interaction in theoretical descriptions of heterogeneous electron transfer.

O 60.12 Wed 17:45 TRE Phy

Dynamic Polymorph Formation of a Trimesic Acid Derivative at Solid-Liquid Interface — •Richa Arjariya[1], Vipin Mishra[1], Gagandeep Kaur[1], Sandeep Verma[1], Markus Lackinger[2], and Thiruvancheril G Gopakumar[1] — [1]Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur, UP-208016, India — [2]Department of Physics, Technical University of Munich, James-Franck-Strasse 1, Garching 85748 and Deutsches Museum, Museumsinsel 1, Munich 80538, Germany

In this work we show the self-assembly of a tricarboxylic acid derivative of trimesic acid (BTA) at heptanoic acid-, nonanoic acid-graphite interface. At both interfaces BTA forms a trimer based-self-assembly, super-flower (SF) pattern. The spontaneously formed SF pattern is observed to be dynamically converting to a dimer-based assembly, chicken-wire pattern (CW), at heptanoic acid-graphite interface while scanning. Interestingly, at nonanoic acid-graphite interface, SF pattern remains stable and not converted to CW pattern. We attribute that the formation energy of both SF and CW patterns is comparable. The difference in the stability of different patterns in heptanoic acid and nonanoic acid is most likely related to the solubility of BTA in these solvents.[1,2] 1) T. N. Ha, T. G. Gopakumar, M. Hietschold, J. Phys. Chem. C, 2011, 115, 21743. 2) M. Lackinger, S. Griessl, W. M. Heckl, M. Hietschold and G. W. Flynn, Langmuir, 2005, 21, 11, 4984-4988

O 61: Focus Session: Frontiers of Electronic-Structure Theory V (joint session O/HL)

Time: Wednesday 15:00–17:30 Location: TRE Ma

O 61.1 Wed 15:00 TRE Ma

Phase transitions in the two-dimensional Su-Schrieffer-Heeger model — •Changan Li[1], Songbo Zhang[2], Sangjun Choi[1], Jan Budich[3], and Björn Trauzettel[1] — [1]Institute for theoretical physics and astrophysics, University of Würzburg, Wuerzburg, Germany — [2]Department of Physics, University of Zürich, Winterthurerstrasse 190 8057, Zürich, Switzerland — [3]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

The 2D Su-Schrieffer-Heeger (SSH) model is endowed with rich topological physics. First we show that the random flux can induce a metal-band insulator transition in the 2D SSH, thus reporting the first example of such a transition. Remarkably, we find that the resulting insulating phase can even be a higher-order topological insulator with zero-energy corner modes and fractional corner charges. Employing both level statistics and finite-size scaling analysis, we characterize the metal-band insulator transition and numerically extract its critical exponent. By proposing another inclined 2D SSH model, a deformed one, we show that a pair of Dirac points protected by space-time inversion symmetry appear in the semimetallic phase. Interestingly, the locations of these Dirac points are not pinned to any high-symmetry points of the Brillouin zone but highly tunable through parameter modulations. Moreover, the merging of two Dirac points undergoes a topological phase transition, which leads to either an anisotropic topological insulating phase or a nodal-line metallic phase.

O 61.2 Wed 15:15 TRE Ma

Ab initio embedding approach for carbon defects in hexagonal boron nitride: A new platform to probe environmental screening — •Danis Badrtdinov[1], Magdalena Grzeszczyk[2], Alexander Hampel[3], Cyrus Dreyer[3,4], Maciej Koperski[2], and Malte Rösner[1] — [1]Radboud University, Nijmegen, The Netherlands — [2]National University of Singapore, Singapore — [3]Flatiron Institute, USA — [4]Stony Brook University, USA

Correlated defects in layered van der Waals hosts hold high promises for realizing quantum technologies, as they allow for various possibilities to control defect properties, e.g., via altering the host thickness or by changing the substrate material. A quantitative description of the defect ground and excited states taking the details of the impurity environment into account is, however, a considerable challenge for conventional density-functional theory (DFT) based methods as the impurities might be correlated and dielectric environmental screening is not fully accounted for in DFT. To tackle these challenges we apply and extend an embedding approach that treat the defect states within exact many-body theory, while DFT is used as a starting point to describe the bulk host material. We study various carbon defects embedded in hexagonal boron nitride (hBN), allowing us to disentangle all mechanisms responsible for the alteration of defect properties including modifications to the impurity structure and changes in the environmental screening upon thinning down the hBN host. Our new embedding approach paves the way for improved identification of defects in layered materials and to tailor their properties.

O 61.3 Wed 15:30 TRE Ma

Nonequilibrium electron dynamics in a two-sites Hubbard model — •Jakub Wronowicz and Yaroslav Pavlyukh — Department of Theoretical Physics, Wrocław University of Science and Technology

Electron dynamics in a two-sites Hubbard model is studied using the nonequilibrium Green's function approach using formalism developed in [1]. We focus on the electron dynamics arising in the adiabatic switching scenario. Many-body approximations are classified according to the channel of the Bethe-Salpeter equation in which electronic correlations are explicitly treated. They give rise to the so-called second Born, T-matrix and GW approximations. In each of these cases, the model is reduced to a system of ordinary differential equations, which resemble equations of motion for a driven harmonic oscillator with time-dependent frequencies. We discuss transient solutions for the off-diagonal density matrix. Analytical result for the steady state in second Born approximation is compared with the exact solution. It is further shown numerically that in the large Hubbard-U limit the T-matrix in the particle-hole channel and spin-adapted GW approximations converge to the same solution.

[1] Y. Pavlyukh, E. Perfetto, and G. Stefanucci, *Photoinduced dynamics of organic molecules using nonequilibrium Green's functions with second-Born, GW, T-matrix, and three-particle correlations*, Phys. Rev. B **104**, 035124 (2021).

O 61.4 Wed 15:45 TRE Ma

Time-linear quantum transport simulations with correlated nonequilibrium Green's functions — •Riku Tuovinen[1], Yaroslav Pavlyukh[2], Enrico Perfetto[3], and Gianluca Stefanucci[3] — [1]Department of Physics, Nanoscience Center, University of Jyväskylä, Finland — [2]Department of Theoretical Physics, Wroclaw University of Science and Technology, Poland — [3]Dipartimento di Fisica, Università di Roma Tor Vergata, Italy

We present a time-linear scaling method for open and correlated quantum systems. The method inherits from many-body theory [1] the possibility of selecting the most relevant scattering processes, thereby paving the way for real-time characterizations of correlated ultrafast phenomena in quantum transport. The open system dynamics is described in terms of an embedding correlator from which the transient current can be calculated via the Meir-Wingreen formula [2]. We efficiently implement the method through a combination with recent time-linear schemes for closed systems [3]. Electron-electron and electron-phonon interactions can be treated on equal footing while preserving all fundametal conservation laws. We employ the method by studying transport of correlated electron-hole pairs in semiconductors [4].

[1] G. Stefanucci and R. van Leeuwen, Nonequilibrium Many-Body Theory of Quantum Systems (CUP 2013).

[2] Y. Meir and N. S. Wingreen, PRL 68, 2512 (1992).

[3] N. Schlünzen, J.-P. Joost, and M. Bonitz, PRL 124 (2020) 076601.

[4] R. Tuovinen, Y. Pavlyukh, E. Perfetto, and G. Stefanucci, arXiv:2211.15635 (2022).

15 min. break

Topical Talk O 61.5 Wed 16:15 TRE Ma

Challenges in modelling correlated electronic matter — •Roser Valenti — Institute of Theoretical Physics, Goethe University Frankfurt, Frankfurt, Germany

The microscopic modelling of correlated electronic matter from first principles poses a fundamental theoretical challenge due to the many-body character of the systems. In recent years there have been a few internationally coordinated efforts in theoretical method development to generate a common platform of benchmarked software tools including dynamical mean field theory and extensions.

In this talk I will present some of the challenges we face in such an endeavour and illustrate them with some examples on models and materials.

Funding from the DFG through QUAST FOR 5249-449872909 is acknowledged.

O 61.6 Wed 16:45 TRE Ma

Electron-Phonon Interactions from DFPT within an All-Electron Framework — •Sebastian Tillack, Pasquale Pavone, and Claudia Draxl — Humboldt-Universität zu Berlin and IRIS Adlershof, 12489 Berlin, Germany

The interplay between electrons and the motions of nuclei in solids, described in terms of phonons, play a crucial role in the modeling of functional materials, particularly for understanding temperature dependent effects. We present an implementation of density-functional perturbation theory (DFPT) within a full-potential all-electron framework as implemented in the code `exciting` [1]. Our implementation allows one to compute phonons as well as the linear response to external electric fields. We use DFPT calculations to study lattice vibrations and electron-phonon interactions (EPIs) by means of many-body perturbation theory in β-Ga_2O_3. The electron self-energy contribution is computed as a function of temperature from which various properties such as quasi-particle energies, electron linewidths, and spectral functions are derived. We further incorporate many-body electron-electron interactions described by the GW method. Beyond that, our work creates the foundation for a fully *ab initio* study of the effect of EPIs on optical excitations.

[1] A. Gulans, et al. J. Phys.: Condens. Matter 26, 363202 (2014).

O 61.7 Wed 17:00 TRE Ma

Calculation of phonon spectra with the FLAPW method using Density Function Perturbation Theory — •Alexander Neukirchen, Christian-Roman Gerhorst, Gregor Michalicek, Daniel Wortmann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Computing phonons applying density functional perturbation theory (DFPT) within all-electron DFT methods is a well-known challenge due to the displacement of muffin-tin spheres and sphere-centered basis functions. In this talk, we present our current results of the phonon dispersion based on our implementation of the DFPT approach in the FLEUR code [1] (www.flapw.de), an implementation of the full-potential linearized augmented plane wave (FLAPW) method. We highlight the good agreement of our preliminary results with phonon dispersions obtained with the finite displacement method for which the FLEUR code has been combined with the phonopy tool (www.phonopy.github.io/phonopy/). We discuss the numerical challenges involved in calculating meV quantites on top of large ground state energies typical for all-electron methods and how we addressed them.

This work has been supported by the Helmholtz Postdoc Programme (VHPD-022) and by the MaX Center of Excellence funded by the EU through the H2020-INFRAEDI-2018-1 767 (Grant No. 824143).

[1] A. Neukirchen, C.-R. Gerhorst, D. A. Klüppelberg, M. Betzinger, D. Wortmann, G. Michalicek, G. Bihlmayer, S. Blügel, to be published.

O 61.8 Wed 17:15 TRE Ma

Electron-phonon interaction using a localized Gaussian basis set — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial mechanism in solid state physics that is responsible for a multitude of phenomena. However, in electronic structure calculations it is usually neglected. We developed an 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.

This implementation circumvents the limiting problems of previous implementations while maintaining a good agreement with the literature. The calculated Fan-Migdal zero-point renormalization of the direct band gap of silicon amounts to about 15 meV compared to 20 meV in the literature. Also the temperature-dependence of the renormalization agrees similarly well.

O 62: Focus Session: Wissenschaftskommunikation / Outreach (joint session HL/O/TT)

Im wissenschaftlichen Umfeld wird Maßnahmen der Öffentlichkeitsarbeit eine zunehmend größere Bedeutung zugemessen, - aus der Gesellschaft heraus und auch durch die großen Fördereinrichtungen und die DPG. Dabei geht es nicht nur um die Ergebnisse der Forschung, sondern auch darum, Prozesse und Methoden von wissenschaftlicher Arbeit transparent abzubilden – eine Aufgabe, die prinzipiell alle Forschenden übernehmen können. In diesem Symposium sollen erfolgreiche Projekte der Wissenschaftskommunikation, insbesondere aus dem Bereich der Festkörperphysik, vorgestellt werden. In ihrer Gesamtheit sollen sie das Spektrum der Wissenschaftskommunikation hinsichtlich des finanziellen und zeitlichen Aufwands aufzeigen und Methoden für unterschiedliche Zielgruppen vorstellen.

So dient diese Session sowohl als Ideengeber und Inspiration als auch als eine Art Netzwerk-Treffen zum Austausch über die Wissenschaftskommunikation in unterschiedlichen Kontexten.

Time: Wednesday 15:00–18:30 Location: POT 81

Invited Talk O 62.1 Wed 15:00 POT 81

experimentamus! Forschendes Lernen von Physik und Chemie in der Grundschule — •Sebastian Schlücker — Universität Duisburg-Essen, Campus Essen

Der Sachunterricht in der Primarstufe ist ein Konglomerat aus allen Natur- und Gesellschaftswissenschaften, erst in der Sekundarstufe findet eine Aufspaltung in die einzelnen Fächer statt. Zudem unterrichten viele Grundschul-Lehrkräfte fachfremd. Auch der Zeitaufwand für die Vorbereitung von Experimenten ist nicht unerheblich. Wie also kann man trotz dieser Hürden kindgerechte physikalische und chemische Experimente bereits in der Grundschule einführen?

Ich berichte aus 10 Jahren Erfahrung mit dem Projekt experimentamus!. Dabei handelt es sich um einen Kanon aus ca. 40 Experimenten für die Klassen 2 bis 4, welcher die Themen Licht, Wärme, Magnetismus, Wasser, Luft, Feuer und Elektrizität mit einem kindgerechten Alltagsbezug abdeckt. Anstelle des darlegenden Lernens wird auf das Forschende Lernen gesetzt: Frage - Hypothese - Experiment - Beobachtung - Erklärung; diese fünf Stationen des wissenschaftlichen Erkenntnisprozesses werden immer wieder durchlaufen. Ganz im Sinne Martin Wagenscheins wird dabei nach der exemplarischen und sokratischen Methode vorgegangen. Die praktische Implementierung umfasst 1. Materialkisten für alle Themen, 2. kompakte und leicht verständliche Informationshefter für die Lehrkräfte, sowie 3. Lernheftchen für alle SuS. Am Ende möchte ich über Erfahrungen und Herausforderungen im Rahmen dieses Projektes berichten und Ideen für eine mögliche weitere Verbreitung vorstellen.

O 62.2 Wed 15:30 POT 81

Internal interfaces - goals and realisation of a scientific image film — •Ulrich Höfer[1,2] and Michael Dürr[2,3] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]SFB 1083, www.internal-interfaces.de — [3]Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, Germany

Funded by the German Science Foundation (DFG), a professional film maker has produced an image film about the research conducted in the Collaborative Research Center SFB 1083 ”Structure and Dynamics of Internal Interfaces”. The six-minute video clip takes the non-specialist on a journey down to atomic scale to show the progress at the forefront of research at solid/solid interfaces. It is not a demanding educational film. Rather, it is a visually stunning piece that looks like science fiction taken straight out of a movie, with tracking shots that take the viewer down to the nanometer scale, with flights through luminous molecules, exotic excitons, and space-filling laser labs. The film also has a very impressive soundtrack. Gustav Holst's (1874-1934) composition ”The Planets” was re-orchestrated especially for this film. It is available on the youtube channel of the DFG (https://www.youtube.com/watch?v=_-mDt0NzHrc). Visitors of Chemikum Marburg can watch the German version on a 4K OLED screen, a device actually based on microscopic processes at interfaces investigated by SFB 1083.

The idea behind the creation of a professional film, its conceptional design and the necessary steps towards its realization will be outlined.

O 62.3 Wed 15:45 POT 81

Outreach activities of SFB 1083 @ Chemikum Marburg — •Christof Wegscheid-Gerlach, Luise Cleres, Ina Budde, Karl-Heinz Muth, and Marion Enssle — Chemikum Marburg / SFB1083

The diffusion of concepts, methods, and visions of the SFB 1083 on Structure and Dynamics of Internal Interfaces into the general public is our general goal. To this end project Ö makes use of the institution Chemikum Marburg e.V., whose basic idea is to fascinate the public excited about natural sciences. The experiments offered here, stand for chemical, biological, pharmaceutical, and physical subjects related with daily phenomena or beyond. We will give an overview about the introduction of basic ideas and methods of SFB 1083 to the public as well as the institution Chemikum Marburg. The contents of the individual offers, such as experiments within the regular workspace, the workshops for the Girls' Day and the compilation of special workshops that are offered to give high-school students an understanding of the research content of the SFB 1083 are presented. An additional topic is the linking of basic research to applications for regenerative energy resources. Hydrogen fuel cells are well-known to the general public and rely on functional internal interfaces. An additional workshop which was prepared in cooperation with the district Marburg-Biedenkopf gives an overview about production, storage, and application of hydrogen as a new energy resource. We will also share various occasions at Chemikum Marburg where further outreach activities represent SFB 1083.

Invited Talk O 62.4 Wed 16:00 POT 81

Under the Microscope – spotlighting materials and nano science — •Svenja Lohmann and Pranoti Kshirsagar — The Science Talk, Germany

Real Scientists Nano is a science communication project dedicated to materials and nano science. Despite the widespread relevance of materials science to everyday life, we feel that dedicated science communication in this area is much rarer than in other fields. Our aim is to provide a platform for active materials and nano scientists to directly communicate their science and life as a scientist to the public. The use of social media thereby provides a very low threshold to science communication as basically the only requirement is to have an account. We have the goal to showcase the scientific community in all its diversity, and so far (12/2022) had guest scientists from more than 30 countries of origin as well as various fields and career stages. The two main pillars of the Real Scientists Nano project are the @RealSci_Nano Twitter account and the Under the Microscope podcast. Our guest scientists are interviewed for one podcast episode, and subsequently get to tweet from the account for one week following the rotation curation concept. We let curating scientist decide for themselves what they would like to tweet about. The form and content therefore vary greatly. Many of our scientists report from their everyday life, and are for example live-tweeting from a conference, uploading videos or photos from the lab or sending the occasional “stuck in meetings, will return later” tweet. Science communication on social media thus gives the opportunity to open a direct and real-time window into the scientist's life.

30 min. break

Invited Talk O 62.5 Wed 17:00 POT 81

Phyphox – A pocketful of physics — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Most smartphones are used to make phone calls, to write short messages, surf the Internet or check e-mails. However, they can do much more: With the help of the integrated sensors and the free app ”phyphox” (abbreviation for Physical Phone Experiments), pupils, students, and teachers and interested others can independently perform and develop physics experiments. For example, the app can use the accelerometer to record pendulum movements and determine the rotational acceleration in a salad spinner, or the air pressure sensor to determine time-resolved differences in altitude and thus the speed of an elevator. The didactic potential of the app is great, as the students are picked up on ground that is very familiar and attractive to them (smartphones) and are introduced to experimental natural sciences in a playful way and with an extremely low barrier (zero cost, i.e. only one click away). The app helps to get students excited about scientific and technical questions and contexts at an early age. The app is available free of charge for Android and iOS (more information can be found at www.phyphox.org). In my presentation, I will go into the concept of phyphox, introduce the range of functions and show a number of application examples.

O 62.6 Wed 17:30 POT 81

Chair PR representative as a doctoral student's secondary task: A field report — •Paula M. Weber, Felix Friedrich, and Manuel Seitz — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Especially in recent years, it has become more important to communicate one's scientific work and methods to the public in order to show that in the scientific world, knowledge can only be created through research and the scientific process. Yet, extra time besides research is often limited and it is thus difficult to get into science communication. In this talk, I would like to present how PhD students can use their interest in science communication to benefit their own research group as a part-time PR representative.

In the first part of my talk, I will report on our efforts to attract new bachelor and master students. This advertising is focused on an audience with a scientific background, such that lab tours and advertising posters may contain scientific language and references. The second part is about communication with the general public, who usually know physics from their school days. Here, I will report on how we presented our research activities at the Night of Science in Physics and at the "Highlights der Physik" in Würzburg.

Working part-time as a PR representative could encourage doctoral students to try their hand at science communication and develop the associated communication skills.

O 62.7 Wed 17:45 POT 81

Real or Fake - A format in science communication that encurages critical thinking — •Tobias Löffler — Institut für Angewandte Physik Düsseldorf

The outreach format “Real or Fake” aims to train the audience in an critical approach to credible-sounding facts.

It is aimed at the general public and specifically at young people. At the same time, it offers an easy introduction for scientists to audience-oriented communication of science on stage. The format can be performed in front of a live audience or as an interactive online event. It has been proven to work as implemented into science festivals, nights of sciences, as a public individual event and also as part of events with constrained settings - such as outreach events at schools or as part of conferences.

"Real or Fake" was developed in 2017 by scientists around the Berlin March for Science who later founded Besserwissen e.V. with the goal to promote the format and support new organisers. I do cooprate with them since 2019 and have organized more than ten "Real or Fake" events since then.

In my talk, I will present the concept and its origins, give an overview of successful events and show what to do and what support one can get, if one wants to organize a "Real or Fake" event.

Invited Talk O 62.8 Wed 18:00 POT 81

Physics for school and the public at the LMU — •Dr. Cecilia Scorza-Lesch — Fakultät für Physik der LMU, München

Germany lives from research and technology. Physics, as the basis of all empirical sciences and technologies, has a very special, fundamental role to play. The Faculty of Physics at LMU, the largest in Germany, comprises nine research areas, three centres and two excellence clusters. In this talk we will present the approach we use to successfully communicate our various topics of modern research, the role of physics in our daily lives and in the fight against global warming to the schools and the public in a participatory way.

O 63: Poster: Data Management

Time: Wednesday 18:00–20:00 Location: P2/EG

O 63.1 Wed 18:00 P2/EG

SciCat - a meta data catalog and research data management system — •Linus Pithan[1], Massimiliano Novelli[2], Dylan McReynolds[3], Laura Shemilt[4], Carlo Minotti[5], Anastasiia Pylypenko[1], Alexander Gerlach[1], Alexander Hinderhofer[1], Stephan Egli[5], Tobias Richter[2], and Frank Schreiber[1] — [1]Uni Tübingen, DAPHNE (DE) — [2]European Spallation Source (DK/SE) — [3]Lawrence Berkeley National Laboratory (USA) (US) — [4]The Rosalind Franklin Institute (UK) — [5]Paul Scherrer Institut (CH)

SciCat is a modern and flexible data catalogue that facilitates research data management on multiple scales and thereby suits the needs of large scale research facilities, individual research groups (e.g. at universities) as well as scientific communities. SciCat [1] was initially built to serve Photon- and Neutron sources (in the beginning developed at PSI and ESS, later suppored by ExPaNDS & PaNOSC and further institutions). Through the engagement of DAPHNE4NFDI (DAta from PHoton and Neutron Experiments) in the SciCat project there are new use cases emerging especially - but not exclusively - for small scale installations. The use of an homogenized interface (API) to create and search datasets SciCat can e.g. also be used as infrastructure backbone for machine learning (ML) projects in communities by serving datasets for validation, testing and training of ML models. On this poster we aim to give an overview on specific use-cases of SciCat within DAPHNE, which may serve as blueprints to use SciCat also in other scientific communities.

[1] http://scicatproject.github.io, http://github.com/SciCatProject

O 63.2 Wed 18:00 P2/EG

A local solution for automated data acquisition and storage in catalysis — •Abdulrhman Moshantaf[1], Mike Wesemann[1], Patrick Oppermann[1], Heinz Junkes[1], Robert Schlögl[1,2], and Annette Trunschke[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (Germany) — [2]Max Planck Institute for Chemical Energy Conversion, Mühlheim 45470 (Germany)

In order to solve the current challenge in catalysis research in the development of new, scalable catalysts for hydrogen-based future technologies, a better integration of theory and experiment is required. The necessary data exchange demands extensive digitalization in catalysis. Experimental data must be generated reproducibly and with sufficient diversity, and must be available in machine-readable form. Artificial intelligence can then contribute to the discovery of correlations. We have developed a concept for a local data infrastructure and implemented it in a catalysis laboratory. In research projects, handbooks are written (preferably in machine-readable form) detailing how experimental data are obtained, including the definition of benchmark catalysts. To implement the concept of handbooks, automated systems for data acquisition and storage have been designed. Such a system consists of (i) EPICS for communication with devices and data acquisition, (ii) a database (archive), (iii) an archiving appliance for storing time series, (iv) Phoebus for creating graphical user interfaces, (v) Python/Bluesky/Jupyter notebooks for creating automations and evaluations, and (vi) S3 storage for long-term storage.

O 64: Poster: Graphene

Time: Wednesday 18:00–20:00 Location: P2/EG

O 64.1 Wed 18:00 P2/EG

An STM and XPS study of graphene on Rh (111) as a substrate for on-surface assembly of Pt-complexes — •Majid Shaker, Natalie J. Waleska, Simon Jaekel, Eva Marie Freiberger, Valentin Schwaab, Felix Hemauer, Rajan Adhikari, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, Erlangen 91058, Germany

Single platinum atoms have interesting properties and can play an important role in on-surface catalysis. One route to prepare small Pt nanoclusters or even single isolated Pt atoms is to deposit small amounts of Pt on the Moiré structure of 2D materials on lattice-mismatched transition metal surfaces. Such Moiré patterns e.g. of graphene can act as template for the formation of NCs with a narrow size distribution. In this study, a monolayer of graphene was successfully grown on the surface of a Rh(111) single crystal from ethylene (C2H4) as precursor under ultra-high vacuum (UHV). Very small Pt NCs (down to individual atoms) were formed in the valleys of graphene to further act as a transition metal center for the formation of metal complexes by providing appropriate ligands. Scanning tunneling microscopy and synchrotron radiation-based X-ray photoelectron spectroscopy were employed to evaluate the formed inorganic complexes.

We thank Helmholtz-Zentrum Berlin for allocation of synchrotron-radiation beamtime and the BESSY II staff for support during beamtime. This work was funded by the DFG through SFB 953.

O 64.2 Wed 18:00 P2/EG

Graphene on Ru(0001): Layer-Specific and Moiré-Site- Dependent Phonon Excitations — Johannes Halle, Nicolas Néel, •Rebecca Cizek, and Jörg Kröger — Technische Universität Ilmenau

Graphene phonons are excited by the local injection of electrons and holes from the tip of a scanning tunneling microscope. Despite the strong graphene-Ru(0001) hybridization, monolayer graphene unexpectedly exhibits pronounced phonon signatures in inelastic electron tunneling spectroscopy. Spatially resolved spectroscopy reveals that the strength of the phonon signal depends on the site of the moiré lattice with a substantial red-shift of phonon energies compared to those of free graphene. Bilayer graphene gives rise to more pronounced spectral signatures of vibrational quanta with energies nearly matching the free graphene phonon energies. Spectroscopy data of bilayer graphene indicate moreover the presence of a Dirac cone plasmon excitation.

O 64.3 Wed 18:00 P2/EG

DFT study on the ORR mechanism on carbon nitride materials — •Jana Koenigsdorff, Changbin Im, Björn Kirchhoff, and Timo Jacob — Ulm University, Institute of Electrochemistry, D-89081 Ulm

Polymeric carbon nitrides (PCNs) have rapidly gained attention over the last years due to their promising physicochemical properties.[1] With their adjustable narrow bandgap and high visible light responsivity, PCNs are considered as promising potential photo-(electro)-catalysts for various industrial processes such as H_2O_2 formation or CO_2 reduction.[2][3] However, numerous structural and photophysical properties of this material class are not completely understood and hinder in-depth comprehension of the reaction pathways.[2] Most simulation studies that attempted to gain a deeper insight into the reaction mechanisms were based on simple, highly ordered PCN models.[1] However, PCNs obtained by thermal processes often exhibit inhomogeneity and a variety of micro-structural motifs.[2] In this study, we therefore perform DFT calculations to investigate the mechanism of H_2O_2 formation with various PCN models of different degrees of condensation and structural composition in order to screen a wide range of adsorption sites. We are convinced that with this approach, we can establish structure-reactivity relationships that can be used to derive understanding-driven material optimization strategies.

[1] Wei, Z. et. al., *Energy Environ. Sci.* **11** (2018) 2581 - 2589. [2] Lau, V. Lotsch, B., *Advanced Energy Materials* **12** (2022) 2101078. [3] Xia, Y. et. al., *ChemSusChem* **13** (2020) 1730 - 1734.

O 64.4 Wed 18:00 P2/EG

Electronic magneto-transport in epitaxial graphene covered with Bi(110) islands — •Sergii Sologub[1,2], Julian Koch[2], Chitran Ghosal[2], and Christoph Tegenkamp[2] — [1]Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv — [2]Institut für Physik, TU Chemnitz, Reichenhainerstr. 70, 09126 Chemnitz

Magneto-conductance and Hall voltage of epitaxial graphene formed on SiC and covered with ultrathin Bi islands were measured within the range of ±4 T. The structure and morphology of Bi coverages of average thickness up to 4 bilayers, MBE-grown at RT as well as after-annealed, were determined by SPA-LEED and STM techniques. The coverage was found to consist of needle-like (110) islands with “magic” widths and thicknesses.

The analysis of the low-field part of the magneto-conductance reveals a transition from weak-localization (WL) to weak antilocalization (WAL) with increasing Bi coverage and allows to characterize the scattering of conduction electrons by determining electron scattering lengths, namely inelastic-dephasing, intervalley and intervalley symmetry breaking ones. The correlation of the average sizes of and distance between Bi(110) islands for different coverages with the characteristic lengths demonstrate the role of electron scattering on edges and within the islands in the WL-WAL transition. Calculated dependencies of Hall and magneto-resistance allow determining changes of the electron density induced by Bi adsorption and reveal the contribution of electron-electron interaction in electronic transport.

O 64.5 Wed 18:00 P2/EG

Organic Molecules on Graphene grown on a Pt(111) surface — •Shilpa Panchami Raj, Christophe Nacci, and Leonhard Grill — University of Graz

Graphene, a flat monolayer of carbon atoms with two-dimensional honeycomb lattice, exhibits unique properties. If grown on a Pt(111) surface, only weak interaction is found between the substrate and the graphene sheet. This renders it an interesting system to decouple organic molecules on the graphene layer from the metal underneath as they might preserve their electronic structure In this work, we present a scanning tunneling microscopy (STM) study under ultrahigh vacuum (UHV) with the deposition of different organic molecules on graphene that was epitaxially grown on a Pt(111) substrate. Experiments were done at cryogenic temperatures of 5 K, which allows to image single molecules in a stable fashion and also to manipulate them with the tip of the STM in a controlled way. Adsorption properties of the molecules are studied in view of the characteristic Moiré pattern of the graphene/Pt(111) system. Moreover, first attempts will be presented how chemical reactions can be induced on this system.

O 64.6 Wed 18:00 P2/EG

Electronic band structure of Pb intercalated graphene on SiC and the influence of electron doping — •Bharti Matta[1], Philipp Rosenzweig[1], Kathrin Küster[1], Craig Polley[2], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]MAX IV Laboratory, Lund University, Fotongatan 2, Lund 22484, Sweden

Intercalation is a powerful way of modifying the properties of epitaxial graphene and stabilizing two-dimensional (2D) intercalant layers at the graphene/SiC interface. In this work, we show that the charge neutrality of Pb intercalated quasi-freestanding monolayer graphene on SiC involves charge transfer from both the intercalant and the substrate. Synchrotron based angle resolved photoelectron spectroscopy measurements demonstrate the (1×1) order of the Pb layer with respect to SiC. The interlayer bands cross the Fermi level, confirming the metallic nature of intercalated Pb. Furthermore, constant initial state mapping shows no dispersion of the Pb bands with photon energy, proving the 2D nature of the intercalant layer. Polarization dependent measurements retrieve a mainly in-plane orbital character for the Pb band branches closer to the Fermi energy. Potassium deposition induces strong n-doping in the graphene layer ($E_D \approx 1.1$ eV). However, the Pb bands do not show any noticeable change, which suggests that the charge transfer from the potassium layer occurs predominantly into the graphene. Supported by DFG through FOR 5242.

O 64.7 Wed 18:00 P2/EG

Terahertz harmonic generation from graphite pencil drawings — •Atiqa Arshad, Segey Kovalev, and Jan Christoph — Helmoltz Zentrum Dresden (HZDR)

Harmonic generation is a general characteristic of driven nonlinear systems. It can serve as an efficient tool for investigating the fundamental principles that govern the underlying ultrafast nonlinear dynamics. Here we report on terahertz third harmonic generation (THG) from graphite pencil drawings on paper. We demonstrate that the terahertz(THz)-THG efficiency at an excitation frequency of 0.5 THz in graphite is comparable to that of single-layer graphene pump field strengths on the order of 100 kV/cm-1. The THG efficiency in graphite exhibits a significantly less pronounced saturation behavior at high incident fields and thus may even surpass that of graphene at extreme pump field strengths. The less pronounced saturation can be attributed to more efficient heat dissipation in multilayer graphite flakes compared to single-layer graphene. The feasibility of using easy-to-produce graphite-based structures opens up new possibilities for highly accessible, modifiable, and nearly cost-free THz frequency multipliers. Besides the implementation of graphite-based THz frequency converters, the developed technique could be used for nonlinear THz imaging, offering the possibility to image graphite drawings covered by other materials.

O 64.8 Wed 18:00 P2/EG

In-situ monolayer graphene growth on Ru(10$\bar{1}$0): an electron microscopy study — •Cathy Sulaiman, Lukas Schewe, Lars Buss, Moritz Ewert, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany

During the last decade, the controlled growth of monolayer (MLG) and bilayer graphene has extensively been studied on the hexagonal Ru(0001) surface, which is a system that is known to form strong chemical bonds at the metal-graphene interface. Yet, little attention was paid to the influence of the substrate orientation that was demonstrated to have a significant impact for graphene growth on the Ir(001) and Ir(111) surfaces, the latter exhibiting a weak coupling between the graphene and the support. Therefore, in this study we have grown graphene on the rectangular Ru(10$\bar{1}$0) surface by segregation and ethylene-supported chemical vapor deposition. A photoemission and low-energy electron microscope (PEEM & LEEM) has been utilized to directly characterize the MLG growth process with respect to variations in substrate temperature and step orientation. The expansion of the MLG islands is compared to the well-established carpet-growth mode on the Ru(0001) surface. These results have been complemented by probing of the occupied and unoccupied electronic structure of the islands using PEEM and intensity-voltage LEEM. Furthermore, the existence of two preferential surface reconstructions is identified via micro-illumination low-energy electron diffraction (LEED), whose spatial distribution is revealed by employing dark-field LEEM imaging.

O 64.9 Wed 18:00 P2/EG

Band structure and charge carrier dynamics of a Pb-intercalated graphene sheet on Ni(111) — •Eva Sophia Walther[1], Katharina Hilgert[1], Christina Schott[1], Sebastian Hedwig[1], Ka Man Yu[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OP-

TIMAS, RPTU Kaiserslautern, Germany — [2]Institute of Physics, Material Science in Mainz, JGU Mainz, Germany

The discovery of graphene acted as a starting point for the vast research field of 2D materials. However, on metal surfaces, most of the enthusiasm for exploring graphene's unique properties has been tempered by the strong interaction with its substrate, which results in severe changes in its electronic properties. One way to reduce the graphene-surface interactions is the intercalation of heavy metal atoms between the graphene and the underlying substrate. In our work, we use the highly reactive Ni(111) surface as a graphene substrate. On this surface, the linear dispersion of the Dirac cone is severely distorted and the K-point is located far below the Fermi energy. Here, we will show that Pb intercalation recovers the linear dispersion of the free-standing graphene. Using time- and momentum-resolved photoemission, we will further determine the influence of the Pb intercalation for the ultrafast charge carriers dynamics at the K-point of the Gr/Ni(111) interface.

O 64.10 Wed 18:00 P2/EG

Controlled fabrication of the graphene/Mn_5Ge_3 interface via Mn intercalation — •Vivien Enenkel[1], Yuriy Dedkov[2], Elena Voloshina[2], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, Universtätsstraße 10, 78457 Konstanz, Germany — [2]Department of Physics, Shanghai University, 99 Shangda Road, 200444 Shanghai, China

Mn-based intermetallic compounds have recently been in focus of intensive research owing to their outstanding magnetic properties. In particular, epitaxial Mn_5Ge_3/Ge interfaces [1] are regarded to have the potential for the realization of efficient spin injection and manipulation in semiconductor structures compatible with the existing Si technology. Furthermore, for graphene on Mn_5Ge_3 an exchange splitting of the π states is predicted, with the two spin channels exhibiting a large difference in charge carrier mobility [2]. Here, we report on the fabrication of epitaxial graphene/Mn_5Ge_3 by Mn-intercalation at the graphene/Ge(110) interface, initially prepared by atomic carbon deposition on Ge(110) [3]. Depending on the sample temperature different phases can be generated, including Mn_5Ge_3, whose structure and electronic properties are studied by low-temperature scanning tunneling microscopy and spectroscopy.

[1] Y. Dedkov *et al.*, J. Appl. Phys. 105, 073909 (2009).
[2] E. Voloshina and Y. Dedkov, J. Phys. Chem. Lett. 10, 3212 (2019).
[3] J. Tesch *et al.*, Carbon 122, 428-433 (2017).

O 64.11 Wed 18:00 P2/EG

Force-Field Development for Graphene-Graphite Water Systems — •Otto Schullian and Roland Netz — Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

The wetting behavior of water on graphene/graphite surfaces is strongly dependent on the force fields chosen for the water-carbon interaction. Previously developed force fields were optimized to reproduce a specific contact angle for water on graphite (in the range of 85° to 95°). However, experiments show that the contact angle for water on graphite depends strongly on the preparation of the surface; they suggest that freshly exfoliated graphite has a surprisingly hydrophilic contact angle of 60°±13°, whereas old and potentially contaminated graphite surfaces are much more hydrophobic. For graphene the variance in contact angle is even more dramatic, ranging from 10° to 127°.

Here, we simulate contact angles for a range of water-carbon interaction strengths for one to five layers of graphene to provide the necessary parameters for a whole range of contact angles (30°-115°). In this way, one can tune the wetting behavior in simulation. From our results, we see that the graphene with no underlying support has a contact angle 2°-20° higher than the corresponding graphite system depending on the interaction strength. In addition, we investigate the frequency-dependent friction on flat graphene and graphite as a function of the interaction strength and the number of graphene layers via the Green-Kubo relation including a hydrodynamic correction.

O 64.12 Wed 18:00 P2/EG

Raman features of graphene and Weyl semimetals beyond the standard nonadiabatic theory — •Nina Girotto and Dino Novko — Institute of Physics, Zagreb, Croatia

Although graphene has already been thoroughly studied with Raman spectroscopy, there still exists a disagreement about the broadening mechanisms of the E2g mode and its actual temperature dependence [Nano Lett. 10, 466 (2010)]. Along with the importance of the nonadiabatic effects in graphene, higher order electron-phonon scattering processes also significantly impact the phonon spectrum. Specifically, the electron-phonon-induced lifetime and energy renormalization of the electron-hole pair excitations bring additional temperature dependence in the electron-coupled phonon modes and their corresponding linewidths. The nonadiabatic theory relying on first principles calculations, developed in [Phys. Rev. B 98, 041112(R) (2018)], is here successfully applied to graphene in various doping regimes and to Weyl semimetals, which contain a 3-dimensional analog of Dirac points in the electron band structure and are, therefore, excellent candidates for achieving a nonadiabatic regime.

O 65: Poster: Topology and Symmetry-Protected Materials

Time: Wednesday 18:00–20:00 Location: P2/EG

O 65.1 Wed 18:00 P2/EG

Topological insulator Bi2Se3: the effect of doping with Fe, Ru, Os, and Mo — •Frantisek Maca[1], Stanislav Cichon[1], Vaclav Drchal[1], Katerina Horakova[1], Irena Kratochvilova[1], Jan Lancok[1], Vladimir Chab[1], Patrik Cermak[2], Cestmír Drasar[2], and Jiri Navratil[2] — [1]Institute of Physics CAS, Praha, Czech Republic — [2]University of Pardubice, Pardubice, Czech Republic

Doping is one of the most suitable ways of tuning the electronic properties of topological insulators (TI) and a promising means of a band gap opening. We report a reliable method for preparation of high-quality single crystal substrates Bi2Se3 containing anti-site defects and vacancies and doped with VIIIB and VIB columns elements.

We combine experimental (XPS, ARPES) and theoretical (ab initio) methods to analyze the electronic properties and chemical states of atoms and defects in the substitutional position in TI that can be achieved using the free melt crystallization method of the sample growth. Doping introduced change in the position of Dirac cone is shown and discussed.

O 65.2 Wed 18:00 P2/EG

Green's functions formulation of Floquet topological invariants — •Marcus Meschede, Helena Drüeke, and Dieter Bauer — University of Rostock

Floquet topological insulators (FTIs) allow for topological protection through their time evolution as opposed to static topological insulators, which are only protected by their band topology. FTIs have become ubiquitous in the pursuit of realizing new phases of matter. In general, the momentum-dependent quasi-energy spectrum of single-particle time evolution operators or, equivalently, Floquet Hamiltonians is used to classify the band topology. In the presence of many-particle interactions, this single-particle picture breaks down. In order to overcome this issue, topological invariants of static systems have been formulated through their single-particle Green's functions. [1,2] We expand on this work by calculating Floquet topological invariants through their Floquet Green's function. As there is much experimental work on realizing FTIs, we hope to provide another tool to determine the topological properties of these systems through their bulk spectral function.

[1] Gurarie, V. "Single-Particle Green's Functions and Interacting Topological Insulators." Physical Review B 83, 085426 (2011).

[2] He, Yuan-Yao, Han-Qing Wu, Zi Yang Meng, and Zhong-Yi Lu. "Topological Invariants for Interacting Topological Insulators. I. Efficient Numerical Evaluation Scheme and Implementations." Physical Review B 93, 195163 (2016).

O 65.3 Wed 18:00 P2/EG

Interaction-Induced Directional Transport on Driven Coupled Chains — •Helena Drüeke and Dieter Bauer — Universität Rostock

We examine whether interaction between particles may introduce (topologically protected) directional transport in a driven two-particle quantum system. As a simple example, we consider two one-dimensional chains of equal length, each with one particle. The two particles interact but stay on their respective chain. The particles move alternatingly and without a preferred direction.

Without interaction between the particles, they each diffuse along their chains. Interaction between them suppresses this diffusion. With the proper timing of their alternating movement, the particles form a bound doublon state. Depending on their starting positions, this doublon either remains stationary or moves along the chain. The motion of the doublon consists of alternating, leapfrogging motion of the two particles.

O 65.4 Wed 18:00 P2/EG

Near-field investigation of topologically protected edge states in plasmonic waveguide arrays — •Hans-Joachim Schill, Anna Sidorenko, and Stefan Linden — Department of Physics, University of Bonn, Germany

Light propagation along evanescently coupled waveguide arrays resembles mathematically the dynamics of a lattice Schrödinger equation and is, therefore, ideally suited for simulating condensed matter lattice systems. Here, we report on near-field measurements with scattering-type scanning near-field optical microscopy (s-SNOM) in transmission mode combined with leakage radiation microscopy to investigate topological effects in coupled arrays of dielectric loaded surface plasmon polariton waveguides (DLSPPWs). Specifically, we implement the Su-Schrieffer-Heeger (SSH) model by fabricating arrays of DLLSPPWs with alternating weak and strong couplings. The interface between two topologically distinct domains of the SSH model is known to host a topologically protected edge state. The combination of far- and near-field imaging allows us to investigate the global intensity evolution of the lattice as well as the local amplitude and phase distribution of the edge state.

O 65.5 Wed 18:00 P2/EG

Orbital Protection of a Weyl Nodal line — •Tim Figgemeier[1,3], Maximilian Ünzelmann[1,3], Philipp Eck[2,3], Jakub Schusser[1,3], Jennifer Neu[4,5], Theo Siegrist[4,6], Domenico Di Sante[7], Giorgio Sangiovanni[2,3], Hendrik Bentmann[1,3,8], and Friedrich Reinert[1,3] — [1]EP VII, Universität Würzburg, Germany — [2]ITPA, Universität Würzburg, Germany — [3]Würzburg-Dresden Cluster of Excellence, ct.qmat — [4]NHMFL, Tallahassee, FL, US — [5]Nuclear Nonproliferation Division, ORNL, Oak Ridge, Tennessee, US — [6]FAMU-FSU, Tallahassee, FL, US — [7]Center for Computational Quantum Physics, Flatiron Institute, New York, US — [8]NTNU, Trondheim, Norway

We present a combined soft X-ray angle-resolved photoelectron spectroscopy (SX-ARPES) and density functional theory study on TaAs and NbP. The two compounds are usually known as paradigmatic non-magnetic Weyl semimetals. Here, however, we show that they further host twofold spin-degenerate nodal lines located at the center of a one-dimensional vortex line of Orbital Angular Momentum (OAM). These momentum space vortices can be tracked experimentally by using k_z-resolved dichroic SX-ARPES. The OAM vortex line protects the spin degeneracy against spin-orbit coupling and imparts high topological robustness to the nodal line. In order to investigate the impact of SOC on the degeneracy experimentally, we compare TaAs with NbP, which differ from each other by having a different magnitude of atomic SOC strength.

O 65.6 Wed 18:00 P2/EG

Towards *higher−order* topological corner states in quantum spin Hall insulating heterostructures — •Markus Feld[1,2], Philipp Eck[1,2], and Giorgio Sangiovanni[1,2] — [1]ITPA, Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence, ct.qmat

Real-space obstruction in $\mathbb{Z}_2$ trivial systems is under current investigation as it promotes quantized electronic bulk multipoles. In two dimensions it can stabilize a *higher−order* topological insulator (HOTI) with insulating edges and zero energy in-gap corner states. However the recent analysis for the triangular quantum spin Hall insulator (QSHI) indenene has extended the concept of real-space obstruction to $\nu = 1$ phases [1].

We show that this is in contrast to the well established large-gap QSHI bismuthene [2], where the Wannier functions center on the atomic lattice sites. Here we present an *ab initio* based study, where we address the edges and corners of obstructed and non-obstructed interfaces by considering heterostructures of indenene and bismuthene.

[1] P. Eck et al., Phys. Rev. B **106**, 195143 (2022)

[2] F. Reis et al., Science **357**, 287 (2017),

O 66: Poster: Scanning Probe Microscopy with Quartz Sensors

Time: Wednesday 18:00–20:00 Location: P2/EG

O 66.1 Wed 18:00 P2/EG

Atomically Precise Synthesis and Characterization of Heptauthrene with Triplet Ground State — Xuelei Su[1], Can Li[2], •Qingyang Du[1], Kun Tao[3], Shiyong Wang[2], and Ping Yu[1] — [1]School of Physical Science and Technology, ShanghaiTech University, 201210 Shanghai, China — [2]Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Shenyang National Laboratory for Materials Science, School of Physics and Astronomy and Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai 200240, China — [3]Key Lab for Magnetism and Magnetic Materials of Ministry of Education, Lanzhou University, 730000 LanZhou, China

Heptauthrene, one of the most well-known structures, is a benzene-fused bisphenalenyls in mirror symmetry with triplet ground state. However, it is difficult to synthesize heptauthrene without any substituents due to its high activity. Owing to the development of on-surface synthesis, it is possible to obtain highly active species with properly-designed precursors. Here, we combined in-solution and on-surface synthesis to achieve unsubstituted heptauthrene, whose chemical structure can be characterized with bond-resolved atomic force microscopy. Its triplet ground state is clearly confirmed by the Kondo resonance around zero bias in dI/dV spectra. The response of this Kondo peak to external magnetic field is also detected to verify the high-spin state. We also engineered its spin-state through hydrogen atom addition or dissociation by tip manipulation. Our work provides access to phenalenyl-based structures with high-spin ground states, potentially useful in constructing spin networks.

O 66.2 Wed 18:00 P2/EG

Novel image interpretation methods for high-resolution STM — •Lauri Kurki[1], Niko Oinonen[1], Ondrej Krejci[1], and Adam S. Foster[1,2] — [1]Department of Applied Physics, Aalto University, 00076, Espoo, Finland — [2]WPI Nano Life Science Institute, Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Scanning tunnelling microscopy (STM) functionalized with a CO molecule on the probe apex is a method capable of capturing sub-molecular level detail of the electronic and physical structure of a sample[1]. However, the produced images are often difficult to interpret due to the convoluted nature of the signal. We propose image interpretation tools to extract physical and electronic information directly from STM images using machine learning.

In recent years, there has been rapid development in image analysis methods using machine learning, with particular impact in medical imaging. These concepts have been proven effective also in SPM in general and in particular for extracting physical features from atomic force microscopy (AFM) images[2]. We build upon these models and show that we can extract atomic positions and electrostatics directly from STM images. We further explore how the accuracy of these predictions varies with the use of a simultaneous AFM signal and ultimately establish the limits of the approach in an experimental context.

[1] Shuning Cai, Lauri Kurki, Chen Xu, Adam S. Foster, and Peter Liljeroth. JACS 144 (44), 20227-20231 (2022)

[2] Niko Oinonen, Lauri Kurki, Alexander Ilin, and Adam S. Foster. MRS Bulletin 47, 895-905 (2022)

O 66.3 Wed 18:00 P2/EG

Distance dependence of s- and p-wave contributions in CO-tip STM — •Leonard-Alexander Lieske, Fabian Paschke, Florian Albrecht, and Leo Gross — IBM Research Europe - Zürich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland

Funtionalized tips are frequently used in high-resolution AFM, particularly CO terminated tips, to facilitate atomic resolution [1]. CO functionalized tips can also enhance contrast in STM measurements of ionic resonances, mapping orbital densities [2,3]. For CO tips both s- and p-wave character of the tip contribute to the contrast [3,4,5]. Here, we study the contributions of s- and p-wave character of CO tips as a function of tip height, bias voltage and tunneling current.

[1] L. Gross, F. Mohn, N. Moll, P. Liljeroth and G. Meyer, Science, 325(5944), 1110-1114 (2009).
[2] J. Repp, G. Meyer, S. M. Stojković, A. Gourdon and C. Joachim, Physical Review Letters, 94(2) 026803 (2005).
[3] L. Gross, N. Moll, F. Mohn, A. Curioni, G. Meyer, F. Hanke and M. Persson, Physical Review Letters, 107(8), 086101 (2011).
[4] N. Pavliček, I. Swart, J. Niedenführ, G. Meyer and J. Repp, Phys. Rev. Lett. 110, 136101 (2013).
[5] A. Gustafsson and M. Paulsson, Phys. Rev. B, 93, 115434 (2016).

O 66.4 Wed 18:00 P2/EG

Atomic-scale imaging of individual cyclic oligosaccharides with non-contact atomic force microscopy — •Márkó Grabarics[1,3], Benjamin Mallada Faes[2,3], Alejandro Jiménez-Martín[2], Pavel Jelínek[2], Bruno de la Torre[2], and Stephan Rauschenbach[1] — [1]University of Oxford, Department of Chemistry, United Kingdom — [2]Institute of Physics of Czech Academy of Sciences, Czech Republic — [3]These authors contributed equally.

Carbohydrates, also referred to as saccharides, are a major class of biopolymers that are essential to all known living organisms. While important in a range of biological processes, the structural complexity of carbohydrates poses a challenge to conventional analytical techinques, which often fail to provide unambiguous structural assignment.

We aim to overcome this challenge by imaging single, surface-adsorbed carbohydrate molecules using high-resolution SPM. For these proof-of-concept experiments, β-cyclodextrin was chosen as model compound, a cyclic oligosaccharide consisting of seven glucose units linked together *via* α-1,4-glycosidic linkages. Incompatible with thermal evaporation, the molecules were deposited in ultrahigh vacuum onto close-packed noble metal surfaces using electrospray deposition. STM and non-contact AFM with CO-functionalized tips revealed two distinct adsorption geometries, with the individual glucose units clearly resolved within the macrocycles.

Our results demonstrate the potential of high-resolution SPM for the structural characterization of carbohydrates, opening up novel ways for the analysis of this important class of biomolecules.

O 66.5 Wed 18:00 P2/EG

observation and definition of lipid raft in live MCF-7 cell by AFM — •Hsiang-Ling Chuang[1], Yu-Chen Fa[2], Chun-Hsien Chen[1], Lli-Chen Wu[3], and Ja-An Ho[1,2] — [1]department of chemistry, National Taiwan University, Taiwan 10617. — [2]department of biochemical science and technology, National Taiwan University, Taiwan 10617. — [3]department of applied chemistry, National Chi Nan University, Nantou, Taiwan 54561.

Lipid rafts are composed of cholesterol, sphingolipid, and proteins. Previous studies indicated that resveratrol and fibrinogen can bind to the receptor on alpha-v beta-3 integrin. Through the protein-lipid or protein-protein interactions, drug-bound integrins will aggregate into larger raft blocks with unbound integrins. Due to the limitation of optical microscopy and complicated sample preparation, the techniques on lipid rafts observation have shortages of real-time and original state information. In this study, we explore the application of in-situ atomic force microscope (AFM) for the observation of lipid rafts on the cell surface and the response upon the administration of chemicals in real time. We obtained AFM images of morphology and stiffness of live breast cancer cells (MCF-7) in phosphate buffered saline (PBS), resveratrol and fibrinogen solutions to identify the location, drifting and aggregation of lipid rafts. Via cross-comparison of AFM images, the regions are higher and stiffer than the surrounding cell membranes resemble the characteristics of lipid rafts. The developed method may be applicable to identify the location of lipid rafts in real-time and allow us to elucidate complex biological systems at the molecular level.

O 66.6 Wed 18:00 P2/EG

Balanced trolling quartz-based sensor with high quality factor used for atomic force microscopy in the liquid — Rui Lin, •Yingzi Li, Jianqiang Qian, and Peng Cheng — School of Physics, Beihang University, Beijing, China

Quartz tuning fork (QTF) has been widely used in atomic force microscopy (AFM) due to its self-sensing property, high quality factor, and high frequency stability. However, owing to the bulky structure and exposed surface electrode arrangement of QTF, the application of quartz-based AFM sensor in the liquid imaging is limited. One way to solve this problem is to coat the QTF with an insulating layer and immerse it into the liquid. However, it would result in a sharp drop of the quality factor and lead to reduction of force detection sensitivity. Here, a high quality factor AFM sensor based on balanced trolling QTF is proposed. Both prongs of the QTF are glued with same tips to make sure high symmetry of QTF, while only one tip is immersed in the liquid. In this configuration, the hydrodynamic interaction can be reduced so that the quartz-based sensor can maintain a high quality factor, which will improve the sensitivity of force detection in the liquid. A theoretical model is presented to analyze the sensing performance of the balanced trolling quartz-based sensor in the liquid. Then, the sensing performance of the sensor is estimated through experimental tests. Finally, the proposed sensor is applied in AFM imaging on different samples in the liquid. The results validate the high quality of the proposed balanced trolling quartz-based sensor and its feasibility of liquid imaging of AFM.

O 66.7 Wed 18:00 P2/EG

AFM characterization of surface metal oxides with an O-terminated copper tip — •Philipp Wiesener, Bertram Schulze-Lammers, Harald Fuchs, and Harry Mönig — Westfälische Wilhelms-Universität, Münster, Germany

Previously we invastigated the performance of various tip terminations, namely Cu-, Xe-, CO-, and O-terminated Cu-tips (CuOx-tips), on the Cu(110)O(2x1) surface with non contact AFM. A direct comparison of the imaging and force-spectroscopy capabilities by these different tip terminations shows, that only for the CuOx-tip a significantly selective force interaction between metal and oxygen atoms can be observerd.

In this work we want to generalize the idea of chemical selective imaging by analyzing a broad spectrum of metal oxide systems with CuOx-tips. We perform constant height measurements over an extendend range of tip sample distances and analyze surfaces that posses varying relative heights of metal and oxygen atoms to probe possible effects on the chemical selectivity. For an additional contrast analysis we investigate various defects of the metal oxide surfaces and complement our site-selective microscopy with force-spectroscopy measuerements on the observerd metal and oxygen atoms.

The performed measurements can be seen as a first step of developing CuOx-tip AFM imaging as an efficient tool for the surface characterization of metal oxide materials. Subsequently, we want to extend our methodology to more complex surface- and bulk metal oxide systems and relate them with complementary DFT calulations and AFM simulations.

O 66.8 Wed 18:00 P2/EG

On-Surface Synthesis of C144 Hexagonal Coronoid with Zigzag Edges — •Xujie Zhu, Yanan Liu, Weiwen Pu, Fang-Zi Liu, Zhijie Xue, Zhaoru Sun, Kaking Yan, and Ping Yu — School of Physical Science and Technology, ShanghaiTech University, 201210 Shanghai, China

Coronoids as polycyclic aromatic macrocycles enclosing a cavity and they can be also regarded as nanoporous graphene molecules whose electronic properties are critically dependent on the size and topology of their outer and inner peripheries. However, because of their synthetic and characteristic challenges, the extended hexagonal coronoids with zigzag outer edges have not been reported yet. Here, we report the on-surface synthesis of C144 hexagonal coronoid with outer zigzag edges on a designed precursor undergoing hierarchical Ullmann coupling and cyclodehydrogenation on the Au(111) surface. The chemical and electronic structure is unambiguously characterized by bond-resolved non-contact atomic force microscopy and scanning tunneling spectroscopy measurements. In combination with the density functional theory calculations, the result is shown that the HOMO-LUMO energy gap oscillates with the size of the central cavity. Moreover, the values of the harmonic oscillator model of aromaticity suggest that the molecular structure is ideally represented by Clars model. Our results provide approaches toward realizing a hexagonal coronoid with zigzag edges, potentially inspiring fabrication of hexagonal zigzag coronoids with multiple radical characters in the future.

O 66.9 Wed 18:00 P2/EG

Setup of a quartz needle sensor-based nc-AFM/STM operating at millikelvin temperatures — •Sven Just[1,2], Taner Esat[1,2], Denis Krylov[1,2], Peter Coenen[1,2,3], Vasily Cherepanov[1,2,3], Bert Voigtländer[1,2,3], Stefan Tautz[1,2], and Ruslan Temirov[1,2,4] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology — [3]mProbes GmbH, 52428 Jülich, Germany — [4]Institute of Physics II, University of Cologne, 50937 Cologne, Germany

A non-contact (nc) atomic force microscope (AFM) is developed for operation in ultra-high vacuum at a base temperature of 300 mK. The AFM is based on an ultra-compact quartz needle sensor oscillating at 1 MHz with a $7.5\,\mu$m thick tungsten tip glued to one end of the needle allowing for simultaneous operation of AFM and STM [1]. Nanopositioners with resistive readout and a scanner with a large low-temperature scan range of $30 \times 30\,\mu m^2$ are used. Additionally, HF wiring for an antenna and a capillary for supply of gases, both close to the junction, are provided. The AFM setup is mounted on a removable insert (mK-stick) for usage in an existing millikelvin system based on adiabatic demagnetization refrigeration (ADR) [2]. Due to the modularity of the mK-sticks a quick exchange is possible without any need for warming up the LHe cryostat.

[1] I. Morawski et al., Rev. Sci. Instrum. **81**, 033703 (2010)

[2] T. Esat et al., Rev. Sci. Instrum. **92**, 063701 (2021)

O 66.10 Wed 18:00 P2/EG

Electrostatic Discovery Atomic Force Microscopy — Niko Oinonen[1], •Chen Xu[1], Benjamin Alldritt[1], Prokop Hapala[2], Filippo Federici Canova[1,3], Fedor Urtev[1,4], Shuning Cai[1], Ondřej Krejčí[1], Juho Kannala[4], Peter Liljeroth[1], and Adam S. Foster[1,5] — [1]Department of Applied Physics, Aalto University, 00076 Aalto, Espoo, Finland — [2]FZU - Institute of Physics of the Czech Academy of Sciences, 182 21 Prague 8, Czechia — [3]Nanolayers Research Computing Ltd., London N12 OHL, United Kingdom — [4]Department of Computer Science, Aalto University, 00076 Aalto, Espoo, Finland — [5]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

While offering high resolution atomic and electronic structure, scanning probe microscopy techniques have found greater challenges in providing reliable electrostatic characterization on the same scale. In this work, we offer electrostatic discovery atomic force microscopy, a machine learning based method which provides immediate maps of the electrostatic potential directly from atomic force microscopy images with functionalized tips. We apply this to characterize the electrostatic properties of a variety of molecular systems and compare directly to reference simulations, demonstrating good agreement. This approach offers reliable atomic scale electrostatic maps on any system with minimal computational overhead.

O 66.11 Wed 18:00 P2/EG

Building up atomically-precise topological heterostructures in one-dimensional conjugated polymers — •Alejandro Jiménez-Martín[1,2,3], Shayan Edalatmanesh[1,2], Benjamin Mallada[1,2], Héctor González-Herrero[4], David Ecija[5], Pavel Jelínek[1,2], and Bruno de la Torre[1,2] — [1]Czech Advanced Technology and Research Institute (CATRIN), Palacký University, Olomouc, Czech Republic — [2]Czech Academy of Sciences, Prague, Czech Republic — [3]Czech Technical University, Prague, Czech Republic — [4]Universidad Autónoma, Madrid, Spain — [5]IMDEA Nanoscience, Madrid, Spain

The discovery of topological phases in acene-based π-conjugated polymers has been one of the most exciting developments in the field of on-surface synthesis [1]. We recently demonstrated that the topological phase transition can be precisely controlled by the length of the polymer [2], where topologically protected zero-mode states forms at the boundary between two interfaces.

In this contribution, we use such new design criteria for engineering the quantum phase to place edge-gap states at specific sites within a single polymer. We investigate the electronic properties and level of hybridization in close enough topological states depending on their separation by Scanning Tunneling Microscopy and non-contact Atomic Force Microscopy. The results presented here could serve as a blueprint for creating topologically protected quantum spin chains.

[1] B. Cirera, et al., Nano letters 14, (2014).

[2] H. González-Herrero, et al., Advanced Materials 33, (2021)

O 67: Poster: Electronic Structure of Surfaces

Time: Wednesday 18:00–20:00 Location: P2/EG

O 67.1 Wed 18:00 P2/EG

Fermi-level pinning at InP(001):H surfaces — •Rachele Sciotto, Isaac Azahel Ruiz Alvarado, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

Stable InP(001):H surfaces are characterized by fully occupied and empty surface states close to the bulk valence and conduction band edges, respectively [1]. However, photoemission shows a surface Fermi level pinning at midgap energy [2]. In order to resolve that apparent discrepancy, we perform density-functional calculations. Ab initio thermodynamics is used to determine the density of surface defects as a function of temperature and hydrogen pressure. The influence of spin polarization and charging on the electronic properties of the surface defects is studied in detail. It is found that in particular P dangling bonds resulting from H desorption give rise partially filled midgap electronic states that are suitable to explain the experimental findings.

[1] WG Schmidt, et al. Phys. Rev. Lett. 90, 126101 (2003); PH Hahn, WG Schmidt, Surf. Rev. Lett. 10, 163 (2003).

[2] DC Moritz, et al. ACS Appl. Mater. Interfaces 14, 47255 (2022).

O 67.2 Wed 18:00 P2/EG

Dielectric anisotropy of heteroepitaxial GaP/AlP films grown on Si(001) from first-principles calculations — •Max Grossmann and Erich Runge — Technische Universität Ilmenau, Ilmenau, Deutschland

Low-defect III-V semiconductor films grown on Si(001) create new opportunities for cost-effective high-performance photovoltaic and optoelectronic devices. The recent work of Nandy et al. [1] shows a route how to drastically reduce the defect concentration of such structures through a thin GaP/AlP buffer layer. The growth of the latter is best monitored via reflection anisotropy spectroscopy (RAS). The theoretical characterization of RAS spectra is therefore vital for the monitoring of semiconductor growth processes as well as the understanding and improvement thereof. For these reasons we analyse the dielectric anisotropy for the case of a GaP/AlP/Si(001) heterostructure through first-principles calculations and compare them to the RAS measurements of Ref. [1]. [1] M. Nandy, A. Paszuk, M. Feifel, C. Koppka, P. Kleinschmidt, F. Dimroth, and T. Hannappel, A Route to Obtaining Low-Defect III/V Epilayers on Si(100) Utilizing MOCVD, Crystal Growth & Design 21, 5603-5613 (2021), 10.1021/acs.cgd.1c00410

O 67.3 Wed 18:00 P2/EG

Photoemission study of a Te Kagome adatom lattice on Pt(111) — •Nicolai Taufertshöfer[1,2], Begmuhammet Geldiyev[1,2], Maximilian Ünzelmann[1,2], Andreas Raabgrund[3], Tilman Kisslinger[3], Lutz Hammer[3], M. Alexander Schneider[3], Hendrik Bentmann[4], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, JMU Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg — [4]Center for Quantum Spintronics (QuSpin), NTNU Trondheim

Kagome lattices can host a variety of exotic phenomena such as flat bands, topological Dirac physics, or unconventional superconductivity [1]. In this contribution, we investigate the electronic structure of a Pt(111)-(3x3)-Te structure. This phase corresponds to a Kagome adlayer on a strongly reconstructed Pt(111) surface as determined by quantitative LEED-IV and STM. Utilizing angle-resolved photoemission spectroscopy, we find a Fermi surface with a rich structure stemming from a complex manifold of bulk and surface electronic states. Intending to unravel the influence of the Kagome lattice on the surface electronic band structure, we will carefully analyse and discuss our photoemission data. Particular attention will be on the nature of a band located in the close vicinity of the Fermi level at the center of the surface Brillouin zone.

[1] T. Neupert et al., *Nature Physics* **18**, 137-143 (2022)

O 67.4 Wed 18:00 P2/EG

Spin asymmetries in photoemission from $PtTe_2$. — •Muthu Prasath Thirugnanasambandam Masilamani[1], Jakub Schusser[1], Mohammed Qahosh[2], Gustav Bihlmayer[3], Lukasz Plucinski[2], and Friedrich Reinert[1] — [1]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, Jülich, Germany — [3]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, Jülich, Germany

In our recent work [1], we addressed the occurrence of spin-resolved photoemission signal asymmetries in the Weyl type-II semimetal candidate WTe_2. Here, we aim to understand the asymmetric spin texture of electrons photoemitted from surface and bulk states and its relation to the initial state of type-II Dirac semimetal $PtTe_2$ with photon energy of $h\nu = 21.22$ eV at room temperature and at 50K. Our spin- and angle-resolved photoemission data were augmented by the one-step model of the photoemission within the spin-polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) Green's function method of the Munich band structure software package. In order to extract information about the different contributions to the resulting spectral weight and spin polarization, the matrix-element used in our one-step model of photoemission calculations includes all experimental parameters such as photon energy, light polarization and geometry configurations.

[1] T. Heider et al., arXiv:2210.10870 (2022).

O 67.5 Wed 18:00 P2/EG

Quasiparticle lifetime and formation of electronic states at Tellurium–metal interfaces — •Begmuhammet Geldiyev[1,3], Maximilian Ünzelmann[1,3], Philipp Eck[2,3], Domenico Di Sante[2,3], Giorgio Sangiovanni[2,3], Thomas Fauster[4], Hendrik Bentmann[1,3], and Friedrich Reinert[1,3] — [1]Experimentelle Physik 7, Universität Würzburg — [2]Theoretische Physik 1, Universität Würzburg — [3]Würzburg-Dresden Cluster of Excellence ct.qmat — [4]Lst. f. Festkörperphysik, Universität Erlangen-Nürnberg

Properties of interfaces between a device material and metallic contacts can decisively influence the resulting device performance. In particular, the formation of electronic interface states (IS) with short lifetimes could speed up the charge carrier injection [1]. In this contribution, we will discuss the formation of IS at Te – noble metal interfaces, i.e., particularly in a suitable model system AgTe / Ag(111) [2]. Utilizing one- and two-photon photoemission, we find that hybridizations between Te-p_z orbitals with substrate bulk and surface states determine the interface electronic structure. Whilst the AgTe valence band states are located almost completely within the AgTe layer, the wave function of the unoccupied state γ, lying 530 meV above E_F within the projected bulk band gap, has a sizable overlap with the substrate states. Evidence is provided by a rather short lifetime $\tau = 31 \pm 3$ fs of γ as well as by light-polarization-dependent measurements revealing the orbital character of the occupied and unoccupied states.

[1] C. H. Schwalb et al., Phys. Rev. Lett. 101, 146801 (2008)

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

O 67.6 Wed 18:00 P2/EG

Accelerating plane-wave-based *ab initio* molecular dynamics by optimization of Fast-Fourier transforms for modern HPC architectures — •Christian Ritterhoff, Tobias Klöffel, Sagarmoy Mandal, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

The most important advantage of plane-wave basis sets is that wave functions can be transformed efficiently from reciprocal to real space and back by using the Fast-Fourier transform (FFT) algorithm. This allows to evaluate the kinetic and potential energy in reciprocal and real space, respectively, where both operators are diagonal. This reduces the computational cost for applying the Hamilton operator from N^2 to $N \log N$. However, the scalability of current FFT libraries is rather limited on today's HPC systems, which offer large numbers of compute nodes, each of them with many cores. Here we present our optimization of the FFTX library of the Quantum Espresso software package. Data distribution and communication patterns have been revised to make optimal use of combined MPI and OpenMP parallelization. Scalability is further increased by combining FFTs into batches and by introducing overlapping computation and communication. We implemented the revised FFTX library in our optimized version of the CPMD code [1], and we demonstrate the achieved acceleration by a series of benchmark simulations.

[1] T. Klöffel, G. Mathias, B. Meyer, Comput. Phys. Commun. **260** (2021) 107745

O 67.7 Wed 18:00 P2/EG

Comparison of machine learning strategies in the high-throughput exploration of $AB\mathrm{O}_2$ delafossites — •Armin Sahinovic, Benjamin Geisler, and Rossitza Pentcheva — Fakultät für Physik, Universität Duisburg-Essen

The advent of machine learning introduced new techniques to considerably expedite materials discovery. This raises a fundamental question about how they balance interpretability versus accuracy. We address this aspect by comparing ensemble-based active learning (AL) of neural networks (NN) [1] and the sure independence screening and sparsifying operator (SISSO) [2] for the prediction of formation energies and lattice parameters in $AB\mathrm{O}_2$ delafossite oxides. To this end, we generate a consistent dataset from first principles. Element embedding is found to be superior to scalar input strategies, e.g., atomic properties. In conjunction with AL, the NNs reach DFT accuracy, allowing for a significant acceleration of high-throughput materials screening. In contrast, the precision of the physically interpretable SISSO descriptors is limited by the high data complexity. We combine $AB\mathrm{O}_2$ infinite-layer, $AB\mathrm{O}_3$ perovskite [1] and the delafossite data to extend the unsupervised AL into the structural space, thereby enhancing the sample efficiency in the spirit of transfer learning. Finally, we compile a phase diagram that compares the relative stability of the three distinct oxide materials classes.

[1] A. Sahinovic and B. Geisler, Phys. Rev. Research 3, L042022 (2021); J. Phys.: Condens. Matter 34, 214003 (2022)

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

O 67.8 Wed 18:00 P2/EG

Spin-polarized very-low-energy electron diffraction from spin-orbit- and/or exchange-influenced targets — •Christoph Angrick[1], Christian Thiede[1], Andre Reimann[1], Annika Henriksen[1], Nicole Mutzke[1], Moritz Ewert[2,3], Lars Buss[2,3], Jens Falta[3], Jan Ingo Flege[2], and Markus Donath[1] — [1]University of Münster, Germany — [2]BTU Cottbus-Senftenberg, Germany — [3]University of Bremen, Germany

Exchange (XC) or spin-orbit (SOC) interaction cause electron scattering from surfaces to be spin dependent. The resulting spin filtering of the scattered electron beam can be used in spin-polarization analyzers. These analyzers are implemented in, for instance, photoemission setups to obtain spin resolution. Therefore, for promising targets, electron reflectivity and resulting spin asymmetry of very-low-energy electrons are measured for a wide range of incident electron energies and angles. By this, the investigated target is put to a test regarding the usability as a scattering target in a spin-polarization analyzer.

Here, several results of SOC- as well as XC-influenced targets are presented. The results of the SOC-influenced targets Au(111), single-layer MoS_2/Au(111) and W(110) [1] are compared with the results of the XC-influenced target Fe(001)-p(1x1)O [2]. Additionally, the influence of SOC interaction in the case of the XC-influenced target is investigated. The spin asymmetry caused by SOC is found to be one order of magnitude smaller than the spin asymmetry caused by XC.

[1] Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020).

[2] Thiede *et al.*, Phys. Rev. Applied **1**, 054003 (2014).

O 67.9 Wed 18:00 P2/EG

Exploring electronic structural properties of Copper(Cu) via Auger Photoelectron Coincidence Spectroscopy — •Swarnshikha Sinha[1,2], Danilo Kühn[1], and Alexander Föhlisch[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — [2]Universtät Potsdam, Institut für Physik und Astronomie

The electronic structure of the 3d transition metals are immensely influenced by many electron effects. Photoemission spectroscopy (PES) and Auger electron spectroscopy (AES) can help to learn about screening processes in core excited states and electron correlations in two-hole final states, respectively.

However, in Cu 3p photoemission and MVV Auger decay, the final state holes are located in the same main shell as the initial vacancy, leading to strong lifetime broadening in the spectra. APECS, can help in reducing lifetime broadening and revealing overlapping spectral features. [1] A comparative study of three different copper surfaces (111,110 and 100) was conducted using APECS, at the COESCA station, UE52 PGM beamline at BESSYII [2].Our results confirm a strong energy sharing between the Photo and Auger electrons [3]and substantial differences in the screening of the final states, leading to different asymmetry of the atomic multiplet peaks in the two-hole spectra of the three Cu surfaces.

[1] H.W. Haak, et al., Phys. Rev. Lett. 41, 1825 (1978) [2] T. Leitner, et al., J. El. Spec. 250, 147075 (2021) [3] E. Jensen, et al., Phys. Rev. Lett. 62, 71 (1989)

O 67.10 Wed 18:00 P2/EG

Improved convergence of the density response function by an incomplete-basis correction — •Jörn Stöhler[1,2], Markus Betzinger[1], Stefan Blügel[1], and Christoph Friedrich[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [2]RWTH Aachen University, Germany

The polarizability (or density response function) is a central quantity in many electronic structure methods, e.g., the *GW* approach, the random-phase-approximation (RPA) total-energy method, the optimized effective potential method, the Bethe-Salpeter approach, Coulomb-hole screened-exchange (COHSEX). In time-dependent perturbation theory, the polarizability can be expressed as a sum over unoccupied states. However, the resulting sum-over-states expression converges very slowly with respect to the number of bands or the basis-set size, in particular, in systems containing localized *d*- and *f*-states. Here, we discuss a method, called incomplete-basis-set correction [1,2], which augments the sum-over-states expression with a numerical solution of the radial Sternheimer equation in the atomic (muffin-tin) spheres. The method is implemented in the `Spex` code within the FLAPW approach. The resulting polarizability shows a considerably improved convergence behavior with respect to the basis set and the number of unoccupied states.

[1] M. Betzinger, C. Friedrich, A. Görling, S. Blügel, Phys. Rev. B **85**, 245124 (2012), *ibid.* Phys. Rev. B **92**, 245101 (2015).

[2] M. Betzinger, C. Friedrich, S. Blügel, PRB **88**, 075130 (2013).

O 68: Poster: Oxide and Insulator Surfaces

Time: Wednesday 18:00–20:00 Location: P2/EG

O 68.1 Wed 18:00 P2/EG

Sub-nanometer depth profiling of native transition metal oxide layers within single XPS spectra — •Martin Wortmann, Dominik Graulich, Natalie Frese, and Timo Kuschel — Bielefeld University, Bielefeld, Germany

Many transition metals form a thin oxide layer of only few nanometers upon exposure to the atmosphere, which affects their interfacial properties. Such native oxide layers are commonly analyzed using photoemission spectroscopy (PES) and X-ray photoelectron spectroscopy (XPS) in particular. The most common method to obtain compositional depth profiles in PES is based on gradual surface ablation by ion sputtering. However, it is known to affect the microstructure of the surface, compromising depth-resolution and compositional accuracy. Other methods such as angular-resolved, energy-resolved, or hard X-ray PES are associated with considerable experimental effort or demands on sample texture. Here we propose a simple and accessible approach for sub-nanometer depth profiling of native metal oxide layers within single lab-XPS spectra. Heavy transition metals usually have multiple orbital energies within the energy range of a lab-XPS giving rise to peak regions at various binding energies. The signal contributions of oxidized and elemental metals can be distinguished by peak deconvolution. The kinetic energy of the photoelectron determines its inelastic mean free path (IMFP) length, which is a measure for the depth from which information is obtained. Different binding energies can thus be assigned to different values for IMFP, so that an oxide concentration profile can be inferred from a single XPS spectrum.

O 68.2 Wed 18:00 P2/EG

Ab-initio investigations of the order of K$^+$ ions on cleaved muscovite mica — •Andrea Conti, Giada Franceschi, Michael Schmid, Ulrike Diebold, and Florian Mittendorfer — Institute of Applied Physics, TU Wien, Wiedner Hauptstrasse 8-10/134, 1040 Vienna, Austria

Model systems based on single crystals can help to provide a better understanding of the chemistry and the catalytic activity of a given oxide surface. In this work, we present DFT calculations on the surface of muscovite mica, a common phyllosilicate whose structure consists of alternating layers of aluminosilicates and K$^+$ ions. This material easily splits into thin K-terminated sheets, yet the atomistic order of the surface K$^+$ ions has been, until recently, unknown [Franceschi *et al.*, *submitted* (2022)]. Calculations, using the “Vienna Ab-initio Simulation Package” (VASP) and the metaGGA (r^{2}SCAN) exchange-correlation functional, indicate a close correlation between the distribution of the surface K$^+$ ions and the arrangements of the subsurface Al^{3+} ions: the K$^+$ ions preferentially occupy the Al-rich rings. In addition, the calculated diffusion barriers suggest that the K$^+$ ions are mobile enough at room temperature to jump to more favorable sites. AFM simulations, using the Probe Particle Model, are in good agreement with the experimental images.

O 68.3 Wed 18:00 P2/EG

Vanadium and iron intermixing in honeycomb oxides on Pt(111) and Ru(0001) — •Piotr 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

Whereas V and Fe are immiscible in bulk-type perovskite oxides, mixed oxide honeycomb layers can be prepared on Pt(111) and Ru(0001) surfaces. Their atomic composition is accessible from bias-dependent STM topographic images, as the Fe ions develop a protruding contrast with respect to V when tunneling into their 3d(z2) orbitals at elevated bias. On Pt(111), up to 50% iron can be incorporated into a V2O3 host oxide, whereby the Fe runs through a series of distinct configurations evolving from isolated ions to pairs in 3rd neighbor positions, short chains of 2nd neighbor Fe and finally ordered (2x2) V/Fe islands separated by domain boundaries. The observed phase behavior can be traced back to attractive Fe-V and repulsive Fe-Fe pair interactions, which have been identified by DFT calculations and enable perfect reproduction of the experimental patterns by means of Monte-Carlo simulations. In contrast, a V/Fe self-organization scheme becomes active on Ru(0001) that only allows for one unique cation arrangement in the honeycomb oxide. DFT finds a layer of interfacial oxygen between Ru(0001) and the oxide film to be responsible for this rigid structural composition.

O 68.4 Wed 18:00 P2/EG

Atomic View on the (111) Surface of a Cu2O Single Crystal: Reconstruction, Electronic Properties and Band Bending Effects — Alexander Gloystein, Jack Creed, and •Niklas Nilius — Carl von Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany

The nature of the (sqrt3xsqrt3)R30° reconstruction of the Cu2O(111) surface has been heavily debated for almost 30 years. This work demonstrates that the nano-pyramidal reconstruction model that was recently developed for Cu2O(111) thin films is valid also for bulk samples. Well-prepared crystals develop a robust (sqrt3xsqrt3)R30° superstructure in electron diffraction, while atomically resolved STM images display extended arrays of trifold symmetric protrusions with 10.5 Å periodicity. Both findings are in perfect agreement with the nano-pyramidal model, in which Cu4O units attach to every third Cu-O six-ring of a Cu-depleted (111) surface. STM conductance spectra reveal the p-type character of the oxide with the valence-band top pinned to the Fermi level. From band-bending effects in the tip electric field, an induced carrier concentration of 6x10^17 cm-3 is determined for the (sqrt3xsqrt3)R30° phase, increasing to 4x10^18 cm-3 on the few (1x1) patches covered with a Cu-poor minority phase. This difference reflects the close interplay between atomic structure, electronic properties and local screening response for a given surface termination.

O 68.5 Wed 18:00 P2/EG

The Surface Chemistry of Hydrated Lime - Wave Op-

tics tested on a Model System — •Nils Schewe[1], Thomas Mayerhöfer[2], Hicham Idriss[1], and Christoph Wöll[1] — [1]Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, 76344, Germany — [2]Institut für Physikalische Chemie, Friedrich-Schiller-Universität Jena, Jena, 07745, Germany

We report on the results of a combined experimental and theoretical study of the interaction of sulfur dioxide with a calcium hydroxide single crystal surface. Our investigation of this model system for flue gas desulfurization and concrete corrosion was carried out on the Ca(OH)2 (001) surface under ultra-high-vacuum conditions. Combining polarization resolved UHV infrared reflection absorption spectroscopy (IRRAS) with calculations based on wave optical considerations, we were able to demonstrate the adsorption behavior and mode of SO2 on this surface. We show, that the preferred angle of adsorption is 23 ° below 65 K. Heating does not lead to reaction, but fully desorbs the formed adsorbate after crystallization between 80 - 100 K. Additionally, we were able to obtain the first low energy electron diffraction (LEED) pattern of an alkaline earth metal hydroxide by using UHV exfoliation for cleaning.

O 69: Poster: Solid-Liquid Interfaces

Time: Wednesday 18:00–20:00 Location: P2/EG

O 69.1 Wed 18:00 P2/EG

Understanding the mechanism of Li-mediated nitrogen reduction reaction — •Yuanyuan Zhou and Jens K. Nørskov — Department of Physics, Technical University of Denmark, Kongens Lyngby, Denmark

Green ammonia production is a key environmental goal. As a crucial step towards this goal, a direct electrocatalytic N_2 reduction (eNRR) by protons and electrons emerges as a highly desirable alternative. However, all pragmatic attempts to develop such an electrochemical route have so far been hindered by invariably low selectivities and large overpotentials. The most reliable method presently is the lithium-mediated eNRR (LiNR) in non-aqueous electrolytes.[J. Choi *et al.* Nat. Commun. 11, 1-10 (2020)] Despite significant progress made to achieve high FE and current density [K. Li *et al.* Science 374, 1593-1597 (2021), S. Li *et al.* Joule, 6, 2083-2101 (2022)], the mechanism of LiNR is yet not fully understood due to so many intricate processes involved ranging from the atomic scale to the macroscopic scale. Moreover, most Li-NRR studies have the limitations of using a sacrificial solvent as proton donors and difficulties in scaling up production in batch reactors. The talk will, address the long-term stability and high activity of PtAu in the HOR process by suppressing the unwanted THF oxidation and improving the tolerance towards CO-poison. Futhermore, the crucial step for achieving an improved understanding the dynamic change of the solid-electrolyte interphase in different LiNR reaction conditions and the effect on the performance.

O 69.2 Wed 18:00 P2/EG

When qualitative do not imply quantitative differences: Analyzing the oxygen reduction reaction using first-principles kinetic Monte Carlo simulations. — •Elia Zonta[1], Younes Hassani Abdollahi[1,2], Karsten Reuter[1], and Sebastian Matera[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Institute for Mathematics, Freie Universitaet Berlin, Germany, Germany

The oxygen reduction reaction (ORR) is one of the major bottlenecks for the efficiency of fuel cell devices. We implemented a first-principles kinetic Monte Carlo model for this reaction on Pt(111) using a mechanism from literature [1]. This model possesses two reaction pathways contributing to the electrochemical current density. Disabling one of these pathways results in an identical simulated Tafel plot for this reduced model, as compared to the original model with both pathways being active. One might conclude that the turned off pathway is effectively inactive also in the original model and, especially, has no impact on the qualitative kinetics. However, a detailed analysis reveals that both models lead to very different surface coverages and, particularly, exhibit different rate-determining steps. Thus, these qualitative microkinetic differences do not lead to any quantitative differences in the macrokinetic behavior.

[1] R.F. de Morais, P. Sautet, D. Loffreda, and A.A. Franco, Electrochim. Acta 56, 10842 (2011).

O 69.3 Wed 18:00 P2/EG

Electric Double Layer effect on outer-sphere benzyl halides electro-reduction mechanism — •Aleksandr Kramarenko[1], Felix Studt[1], and Evgeny Pidko[2] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]TU Delft, Delft, The Netherlands

Electrocatalytic CO2 fixation is one of the most efficient methods of carbon dioxide conversion, which can be carried out at room temperature and pressure. Thus, the fixation of carbon dioxide with electrochemically activated benzyl halides is an environmentally friendly and ambitious method for the synthesis of the most important carboxylic acid derivatives, which are invaluable for pharmaceuticals and fuel production. For these types of processes, electrocatalysis is a key technology, where electrified interfaces are the main object of study and where the electrochemical potential determines the stability of adsorbed particles and the structure of the electric double layer (EDL) on the electrode surface. Therefore, it is important to gain insight into the electrode-electrolyte interface and the rate-determining reaction steps in order to improve electrode material selectivity and product yields. The combination of first principles and molecular dynamics simulations gives us a good understanding at the molecular level of charged interface phenomena and allows us to study elementary chemical processes in detail, which sheds light on how to improve electrocatalytic reactivity.

O 69.4 Wed 18:00 P2/EG

Atomistic electric double layer modeling of water/metal interfaces from AIMD and continuum approaches — •Sung Sakong and Axel Gross — Ulm University, Ulm, Germany

Electrochemical interfaces are typically associated with forming an electric double layer (EDL) whose theoretical modeling requires an appropriate description of the polarization of the electrode and the electrolyte. In principle, ab initio molecular dynamics (AIMD) simulations are the natural choice as they reliably treat the competing water-water and water-metal interactions and explicitly consider the electronic degrees of freedom [1]. However, this approach is computationally still very demanding and only allows simulations of relatively small canonical ensembles for limited simulation times. Thus, there is a need for computationally less demanding but still reliable approaches to model the EDL. By comparing EDL properties calculated from a continuum method based on a grand canonical scheme [2] with ab initio atomistic approaches [3], we will provide an outlook on possible future directions in the EDL modeling [4].

[1] A. Groß and S. Sakong, Chem. Rev. **122** , 10746 (2022).
[2] S. Sakong *et al.*, Curr. Opinion Electrochem. **33**, 100953 (2022).
[3] S. Sakong, A. Groß, Phys. Chem. Chem. Phys. **22**, 10431 (2020).
[4] A. Groß and S. Sakong, Curr. Opinion Electrochem. **14**, 1 (2019).

O 69.5 Wed 18:00 P2/EG

Water/InP(001) from Density Functional Theory — •Isaac Azahel Ruiz Alvarado and Wolf Gero Schmidt — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, Paderborn, Germany

Water adsorption on the In-rich and P-rich InP(001) surface is studied by density functional theory [1]. Single water molecules attach to three-fold coordinated surface In atoms on In-rich surfaces. Dissociative water adsorption is energetically favorable, but hindered by an energy barrier that decreases with increasing water coverage. The oxygen and hydrogen evolution reactions on InP are characterized by overpotentials of the order of 1.7-1.8 and 0.2-0.3 eV, respectively. The In-rich InP surface band edges lie above the redox potential for oxygen and favors hydrogen evolution. Water adsorption is less favorable on P-rich surfaces and characterized by weak physisorption due to charge accumulation between the water O atom and second-layer In surface atoms.

[1] IA Ruiz Alvarado, WG Schmidt, ACS Omega 7, 19355 (2022).

O 69.6 Wed 18:00 P2/EG

CO_2 Electroreduction Reactions at Gold and Copper Elec-

trodes in Ionic Liquids — •Björn Ratschmeier, Gina Ross, and Björn Braunschweig — University Münster, Institute of Physical Chemistry, Münster, Germany

Room-temperature ionic liquids (RTIL) can play a major role in CO$_2$ reduction reactions in mitigation of existing problems of aqueous electrolytes, such as high overpotentials and product selectivity. In this context, we have studied the influence of Au(111), Cu(111) single crystals, as well as Cu enriched Au(111) electrodes prepared by Cu underpotential deposition with Cu coverages of 1/3, 2/3 and 3/3, in 1-butyl-3-methylimidazolium trifluorosulfonylimide [BMIM][NTf$_2$] for CO$_2$RR. For Au and Cu enriched Au electrodes we observed high selectivity for H$_2$ and CO formation, with onset potentials at around -1.0 V vs SHE and a H$_2$/CO syngas ratio between 0.2-0.4, whereas for Cu only H$_2$ and traces of CO were detected until 1.5 V. By increasing the degrees of coverage of Cu on Au, we were able to modulate the syngas ratio to an optimum ratio of about 1.8 for a monolayer of Cu on Au(111), which approaches the ideal ratio of 2 for Fischer-Tropsch synthesis of hydrocarbons.

O 69.7 Wed 18:00 P2/EG

Exploring charge transfer at electrified interfaces via *ab initio* thermopotentiostat molecular dynamics — •Florian Deissenbeck[1], Mira Todorova[1], Christoph Freysoldt[1], Jörg Neugebauer[1], and Stefan Wippermann[1,2] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Philipps-Universität Marburg

Developing accurate simulation techniques to explore and predict structural properties and chemical reactions at electrified liquid/solid interfaces will be critical to surmount materials-related challenges in the context of energy conversion and storage. Exciting progress in recent years allows us now to realistically describe electric fields at charged surfaces from first principles. Building on these techniques, we recently introduced a “thermopotentiostat”: a novel approach to control the electrode potential in molecular dynamics (MD) simulations [1]. We demonstrate how to implement the thermopotentiostat into density-functional codes [2]. Using ab initio thermopotentiostat MD simulations, we explore the splitting of liquid water and charge transfer reactions at electrified Si and Ge surfaces.

[1] F. Deißenbeck, C. Freysoldt, M. Todorova, J. Neugebauer, S. Wippermann, Phys. Rev. Lett **126**, 136803 (2021)

[2] F. Deißenbeck, S. Wippermann, arXiv:2209.04363

O 69.8 Wed 18:00 P2/EG

Density functional calculations of diffusion paths of methyl thiolate on c(2x2)Cl- and Br-covered Cu(100) surfaces — •Falk Wendorff and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

The surface dynamics of methyl thiolate on Cu(100) surfaces has been studied with video-STM in an electrochemical environment by Yang et al. [1]. Here we present density functional calculations for the diffusion paths and diffusion energy barriers using PWscf and PWneb from the Quantum ESPRESSO package [2]. The diffusion path of CH$_3$S$_{ad}$ substitutionally adsorbed on the c(2x2)Cl- or Br-Cu(100) surface without further halogen vacancies has been inspired by the 'rotation' diffusion path of S$_{ad}$ on these surfaces [3]. Additional vacancies in the halogen adlayer enable further diffusion paths of CH$_3$S$_{ad}$ with significantly lower energy barriers. In case of the Cl coadsorbate the barrier decreases from 1.2 eV to 0.7 eV and in case of Br from 1.6 eV to 0.8 eV. The dipole moment change between the adsorption position and the transition state is negative, which is consistent with the experimental observations by Yang et al. that a more positive sample potential leads to a higher energy barrier [1,4].

[1] Y.-C. Yang *et al.*, Langmuir. **28**, 40, 14143–14154 (2012).

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

[3] B. Rahn *et al.*, Angew. Chem. Int. Ed. **57**, 6065 (2018).

[4] M. Giesen *et al.*, Surface Science. **595**, 127–137 (2005).

O 69.9 Wed 18:00 P2/EG

Growth and structure formation of [EMIm][OTf] on Au(111) — Jonas Hauner[1], •Hanna Bühlmeyer[1], Simon Trzeciak[2], Julien Steffen[3], Dirk Zahn[2], Andreas Görling[3], and Jörg Libuda[1] — [1]Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany — [2]Computer Chemistry Center, Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstraße 25, 91052 Erlangen, Germany — [3]Chair of Theoretical Chemistry, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

The growth mechanisms of ultrathin ionic liquid (IL) films have recently received considerable attention. We report on *in situ* studies of 1-ethyl-3-methylimidazolium trifluoromethanesulfonate ([EMIm][OTf]) on Au(111). The IL thin films were prepared by physical vapor deposition and investigated by scanning tunneling microscopy (STM). We carried out measurements at various sample temperatures and coverages, and identified three different surface structures. At low coverage, [EMIm][OTf] tends to exhibit a 2D-glass structure growing close to gold terraces and the elbows of the well-known herringbone structure of Au(111). Oblique and hexagonal structures of the IL are visible at higher coverage. With temperature-dependent measurements, possible phase transitions and melting points of [EMIm][OTf] were investigated. Small glass-like islands of IL melt at 190 - 200 K resulting in a mobile phase of 2D liquid/gas. Islands with highly ordered structures are stable up to 300 K.

O 69.10 Wed 18:00 P2/EG

In situ surface X-ray diffraction studies of Pt(110) — •Finn Schröter[1], Jan Ole Fehrs[1], Timo Fuchs[1], Jakub Drnec[2], Marta Mirolo[2], David Harrington[3], and Olaf Magnussen[1] — [1]Christian-Albrechts Universität zu Kiel — [2]European Synchrotron Radiation Facility — [3]University of Victoria

The surface oxidation of platinum is an important process in the degradation of platinum electrocatalysts in PEM fuel cells, limiting their lifetime. Its atomic-scale mechanism has been addressed in extensive studies by structure-sensitive in situ techniques. However, these studies up to now have been restricted to room temperature, whereas real fuel cells operate at elevated temperatures of 60°C or higher. We here present first temperature-dependent of the surface oxidation of Pt(111) electrodes in perchlorate solution by in situ high-energy surface X-ray diffraction (HESXRD) The measurements were performed at the ID31 beamline of the European Synchrotron Radiation Facility using photon energies of 70 keV. The kinetics of oxidation-induced extraction of Pt atoms out of the surface was quantitatively determined and correlated with the electrochemical charge transfer measured simultaneously in the experiments. The work was funded by the Deutsche Forschungsgemeinschaft via grant 418603497 and the BMBF via project 05K19FK3.

O 69.11 Wed 18:00 P2/EG

The self-assembly process of helical molecules — Thi N. Ha Nguyen[1], F. Günther[2], K. Preis[1], •J. Kelling[1], C. Tegenkamp[1], and S. Gemming[1] — [1]Institut für Physik, TU Chemnitz, Chemnitz — [2]Instituto de Fisica de Sao Carlos, Universidade de S\~{a}o Paulo, Sao Carlos, Brazil; Instituto de Geocincias e Ciencias Exatas, Universidade Estadual Paulista, Rio Claro, Brazil

Helical polyalanine (PA) molecules gathered a lot of interest as the propagation of electrons along the helical backbone structure comes along with spin polarization. Via liquid and solid scanning tunneling microscopy (STM) we studied the ordering of physisorbed and chemisorbed PA molecules on HOPG and Au surfaces. While enantiopure PA molecules adsorb in a hexagonally close-packed structure, we found heterochiral dimers with a rectangular unit cell for DL-PA. Despite the steric hindrance, the packing density of the DL-PA heterophase is increased by 25% compared to the enantiopure PA structure. Apparently, this is achieved by shifting D- and L-PA along their helical axis. Moreover, the alpha-helix structure of the PA molecules seems to be preserved; thus, electrostatic forces indeed play an important role for the formation and stabilization of the helical structure. In parallel, the interactions between PA homo- and heterochiral pairs were analyzed by van-der-Waals-corrected DFT-based tight binding calculations. Denser packing geometries can be reached by heterochiral PA pairs. Second, coarse-grained classical potentials were derived from the DFTB data, and the different PA phases seen in STM were also successfully obtained from Monte-Carlo simulations.

O 69.12 Wed 18:00 P2/EG

DFT calculation of the S$_{\mathrm{ad}}$ diffusion energy barriers on Ag(100) in the presence of Br coadsorbates — •Sönke Buttenschön and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Coadsorbed halides are known to affect the adatom diffusion on metal surfaces [1]. As a prerequisite for theoretical modelling of the S$_{\mathrm{ad}}$ diffusion on Ag(100) as a function of Br coverage, we have calculated the effect of single and multiple Br coadsorbates on the S_{ad} adsorption energy as well as on the energy at the transition geometry along the S_{ad} diffusion path for various Br coadsorbate configurations with Br coverages up to 0.25. The density functional total-energy calculations have been carried through with PWscf and PWneb from the Quantum ESPRESSO package [2]. The dipole moment of S_{ad} is negative. It is larger in magnitude at the transition state (TS) than at the adsorption position. Averaged over the considered S-Br configurations the absolute value of the S_{ad} dipole moment has a tendency to decrease with Br coverage in qualitative agreement with a depolarization model. After similar averaging, for the TS configurations the superposition of individual S_{TS}-Br pair interaction energies tends to overestimate the actual S_{TS}-Br interaction. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), project 504552981.

[1] B. Rahn, O. M. Magnussen, ChemElectroChem **5**, 3073 (2018).

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

O 69.13 Wed 18:00 P2/EG

Correlation between electrostatic and hydration forces on silica and gibbsite surfaces: An Atomic Force Microscopy Study — •Igor Siretanu, Aram Klaassen, and Frieder Mugele — Physics of Complex Fluids Group, MESA+ Institute, Faculty of Science and Technology, University of Twente, PO Box 217, 7500 AE Enschede, The Netherlands

The balance between hydration and Derjaguin Landau Verwey Overbeek forces at solid-liquid interfaces controls many processes, such as colloidal stability, electrochemistry and ion adsorption. Yet, the hydration forces origin and their relation to the surface charge density controlling the continuum scale electrostatic forces are poorly understood. We argue that these two types of forces are largely independent of each other. Here we performed AFM using intermediate-sized tips that enable the simultaneous detection of DLVO and oscillatory hydration forces at the interface between gibbsite:silica-aqueous electrolyte interfaces. We extract surface charge densities from forces using DLVO theory in combination with a charge regulation boundary conditions for variable pHs and salt concentrations. We simultaneously observe both DLVO and oscillatory hydration forces for an individual crystalline gibbsite particle and the amorphous silica for all fluid compositions. While the diffuse layer charge varies with pH as expected, the oscillatory hydration forces are largely independent of pH and salt concentration, supporting our hypothesis that both forces indeed have a very different origin. We rationalize this based on the distribution of OH groups available for H-bonding on the two distinct surfaces.

O 69.14 Wed 18:00 P2/EG

The interfacial (electronic) structure of InP(001) in contact with electrolytes studied via computational Reflection Anisotropy Spectroscopy — •Vibhav Yadav[1], Margot Guidat[1,2], Mario Löw[2], Jongmin Kim[1,2], Holger Euchner[1], and Matthias M. May[1,2] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen — [2]Institute of Theoretical Chemistry, University of Ulm, Germany

Controlling the electrochemical interface of III-V semiconductors is of great relevance for hydrogen production in Photoelectrochemical water splitting devices. Under operating conditions InP surfaces in contact with the electrolyte can undergo polymerization or dissolution, with the possible formation of In-O-In as charge recombination centers [1,2]. In this work, we vary the oxygen adatom coverage on In-rich and P-rich InP(001) surfaces using Density-functional Theory. Furthermore, we show that combining computational and experimental Reflection Anisotropy Spectroscopy has the potential to provide a better understanding of InP surfaces and their (electronic) structure under applied potentials. [1] May MM, Lewerenz HJ, Lackner D, Dimroth F. Hannappel T. Nat Commun 15, 2015, 9 (15), 8286. [2] Löw M, Guidat M, Kim J, May MM, RSC Adv. 2022, 12 (50), 32756.

O 70: Poster: Plasmonics and Nanooptics II

Time: Wednesday 18:00–20:00 Location: P2/EG

O 70.1 Wed 18:00 P2/EG

Phase correction and stability of a Mach-Zehnder interferometer for 2D electronic spectroscopy — •Simon Durst, Sanchayeeta Jana, Christoph Schnupfhagn, and Markus Lippitz — University of Bayreuth

Fluorescence detected 2D electronic spectroscopy (F-2DES) allows the measurement of ultrafast electron dynamics in complex systems, while disentangling this spectral information from energetically similar phenomena, such as molecular vibration.

The technique requires an excitation signal of four time-delayed laser pulses, which we create via a four-arm Mach-Zehnder interferometer. This interferometer receives a single pulse as an input, and, through the use of delay stages and acusto-optical modulators, outputs a desired pulse train with frequency-modulated phase profiles, used for lock-in detection.

When exciting a sample with this pulse train, special attention must be given to the phase relation between the individual pulses. A mismatch or instability in their spectral phase leads to an excitation with pulses of different lengths or unknown delays and will overall worsen the performance of the setup.

Therefore, this poster highlights the techniques and instruments we use to characterize and compensate the relative phase between the different interferometer arms: GVD correction using a spatial light modulator, a prism compressor setup and interferometric delay scans.

O 70.2 Wed 18:00 P2/EG

In-Situ TEM Study of Structural and Optical Changes by Laser-Induced Grain-Growth — •Jakob Hagen, Murat Sivis, and Claus Ropers — Max-Planck-Institute for Multidisciplinary Sciences, Göttingen, Germany

Resonantly excited surface-plasmons (SP) can be exploited in various scientific fields [1] and have thus sparked widespread attention. One major characteristic of these collective free-electron oscillations is the ability to localize and enhance electromagnetic fields beyond the diffraction limit [2]. Here, we created Aluminum nanodiscs by electron beam lithography (EBL), which are poly-crystalline in nature. In general, single-crystalline structures are preferred because high optical quality can be obtained due to the absence of propagation-damping grain boundaries [3]. Using annealing in an ultrafast transmission electron microscope (TEM) with a pulsed laser source, a grain-growth process could be driven where the boundary migration was observed frame by frame. Upon illumination, the number of grains reduced drastically, leading to almost perfect mono-crystals while preserving the shape. In addition, optical characterization of SPs by photon-induced near-field electron microscopy (PINEM) [4] was carried out before and after annealing. Our approach fuses the precise, nanometric positioning from EBL with the benefits of mono-crystalline plasmonics [5].

[1] S. Lal et al., Nat. Photonics 1, 641-648 (2007), [2] K. B. Crozier et al., J. Appl. Phys., 94, 4632 (2003), [3] M. Bosman et al., Sci. Rep. 4, 5537 (2014), [4] L. Piazza et al., Nat. Commun. 6, 6407 (2015), [5] J.-S. Huang, Nat. Commun., 1:150 (2010)

O 70.3 Wed 18:00 P2/EG

Gold nanoparticles as scannable plasmonic light source for STM enabled electroluminescence — •Cinja S. Müller, Berk Zengin, Aleš Cahlík, and Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

The preparation of high quantum yield tips for electroluminescence includes the use of plasmonic metals, by either making tips from wires of coinage metals or coating of tungsten (or Pt/Ir) tips by violent indentation into Au or Ag crystals. While the former appears as the most logical choice, tips made from ductile coinage metals tend to be mechanically unstable. The plunging of tungsten tips into metal substrates, on the other hand, is rather crude and irreproducible. Here, we attempt to use concepts from both extremes by attaching gold nanoparticles (AuNP) onto the apex of tungsten or Pt/Ir tips. We drop-cast commercially available colloidal AuNP onto a graphite substrate from which the AuNP may be transferred to the STM tip by gentle contact. We describe our setup and characterize the electroluminescence using a fiber-coupled single photon counter.

O 70.4 Wed 18:00 P2/EG

Neuromorphic plasmonic computing - Surface plasmon polariton neurons — •Mario F. Pfeiffer[1], Tobias Eul[1], Eva Prinz[1], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, Germany

Today, the classical electronic computer architecture is the limiting factor for faster, and energy efficient data processing. In combination with the rapidly increasing use of artificial intelligence in science and industry, additional approaches for a suitable hardware architecture are necessary. For this reason, neuromorphic photonics 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) combines photonic advantages such as high bandwidth and speed with strong electronic interactions. These properties have the potential to further advance the development of new hardware. Here we present a concept for building an artificial neuron based on SPP interactions. We have designed initial building blocks of the neuron based on finite-difference time-domain simulations of the plasmonic response. Finally, we imaged this response using a photoemission electron microscope.

[1] Shastri, B.J., Tait, A.N., Ferreira de Lima, T. et al., Nat. Photonics 15, 102-114 (2021)

O 70.5 Wed 18:00 P2/EG

Optical writing of switchable mid-infrared surface phonon polariton resonators with the plasmonic phase-change material In_3SbTe_2 — •Luis Schüler, Lukas Conrads, Konstantin Georg Wirth, Matthias Wuttig, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

Chalcogenide-based phase-change materials (PCMs) are prime candidates for active nanophotonics. They can be reversibly switched between an amorphous and a crystalline state, which exhibit a strong contrast in optical and electrical properties [1]. Therefore, PCMs can be used, for example, to tune surface phonon polariton (SPhP) resonances in the infrared [2]. The recently introduced PCM In_3SbTe_2 (IST) possesses a crystalline phase which is metallic in the entire infrared range. It allows for direct writing of arbitrary resonant structures in a dielectric surrounding [3], which could also confine SPhPs in cavities of subwavelength size. However, an investigation of different confined modes in those cavities with IST has not been performed yet. Here, we investigate IST on a SiC substrate. By laser-induced phase switching, we define various SPhP resonator structures, such as circular cavities, and measure their resonant behavior with optical near- and far-field methods. This study is a first step towards rapid prototyping of switchable SPhP resonators of arbitrary shape that could be employed, for example, in chemical sensing and active metasurfaces.

[1] Wuttig, M. et al. *Nature Photonics* **11**, 465-476 (2017).
[2] Sumikura, H. et al. *Nano Letters* **19**, 2549-2554 (2019).
[3] Heßler et al. *Nature Communications* **12**, 924 (2021).

O 70.6 Wed 18:00 P2/EG

Enhanced Second Harmonic Generation from Silver Nanoantennas — •Fabian Scheidler, Johanna Klos, Jessica Meier, Luka Zurak, and Bert Hecht — Nano-Optics and Biophotonics Group, Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Plasmonic gold nanostructures allow to achieve large field enhancement in nanoscale volumes and are therefore appealing to boost nonlinear processes such as second harmonic generation (SHG). Especially intense near-field hot spots emerge in the gaps of symmetric dimer antennas, yet strong SH sources created in the gap region oscillate out-of-phase and thus destructively interfere in the farfield [1]. Introducing local asymmetry by careful design of the antenna gap geometry allows to mitigate the so-called silencing effect and leads to enhanced SHG [2].

In the ultraviolet-visible spectral range, however, the SH efficiency for gold nanoantennas is limited due to high damping below 500 nm. Here we present silver nanoantennas fabricated from epitaxial grown single-crystalline microplatelets to boost SHG below 500 nm, where silver shows significantly less absorption losses compared to gold. The antenna design is optimised for SHG taking into account the linear scattering response with a resonance at the SH.

[1] J. Berthelot et al., Optics express, 20(10), 10498-10508 (2012).
[2] J. Meier et al., arXiv:221014105 (2022).

O 70.7 Wed 18:00 P2/EG

A room temperature tunable scanning fiber Fabry-Pérot cavity microscope — •Lars Denzer, Paul Steinmann, and Stefan Linden — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

Since the technological advancements in the fabrication of ultrasmooth concave fiber surfaces, fiber-based Fabry-Pérot cavities (FFPCs) are a field of ongoing research. Many applications emerged, ranging from light-matter coupling utilizing very small mode volumes over cavity-enhanced sensing, to cavity microscopy. Here, we report on the construction and test of a tunable scanning fiber Fabry-Pérot cavity microscope operating at room temperature. To this end, we fabricated a concave metallic mirror on the facet of an optical fiber. Using a focused CO2 laser beam, we achieve an ultra-smooth Gaussian depression at the fiber facet. Afterwards, the fiber is gold-coated in an evaporation chamber. Coarse tuning of the cavity is possible by the use of a 3D-piezo stage and the cavity length is fine-tuned by a shear piezo. Laterally scanning the cavity enables a mapping of the sample surface. As a first test, we investigate the coupling of a MoSe2 monolayer to the cavity field.

O 70.8 Wed 18:00 P2/EG

Near-field scanning optical microscopy of topologically protected excitons in molecular aggregates — Sidhartha Nayak, Christopher W. Wächtler, and •Alexander Eisfeld — MPIPKS, Dresden, Germany

Delocalized excitonic eignestates of molecular aggregates are responsible for the energy transfer from an incoming radiation into the aggregate. Static disorder, which can arise from an imperfect environment of each molecule, reduces the exciton transport and large disorders can even localize the exciton. It has been shown theoretically that a two-dimensional periodic array of tilted and interacting molecules in a homogeneous magnetic field shows topologically protected edge states [1]. With a scattering scanning near-field optical microscope setup, one can not only record position dependent absorption spectra [2] but also reconstruct the wavefunctions from these specta [3]. We study theoretically the near field spectra of the aforementioned 2D aggregates in which the molecules experience a disordered environment because of the probing metallic tip. Due to the topological protection, the edge states are robust even in the presence of the metallic nanoparticle, such that the spectrum shows clear signatures of these states.

[1] J. Y. Zhou, S. K. Saikin, N. Y. Yao and A. Aspuru-Guzik, *Nature materials* 13, 1026-1032 (2014)
[2] S. Nayak, F. Zheng and A. Eisfeld, *J. Chem. Phys.* 155, 134701 (2021)
[3] F. Zheng, X. Gao and A. Eisfeld, *Phys. Rev. Lett.* 123, 163202 (2019)

O 70.9 Wed 18:00 P2/EG

Nanoantenna Conjugated Graphene Photodetectors — •Abhinav Raina, Mo Lu, Max Reimer, Vasilii Osipov, Klaus Meerholz, and Klas Lindfors — Department für Chemie, Universität zu Köln, 50939, Köln, Germany

Optical communications is a technology that utilizes light for the wireless transduction of signals. Over the past few decades, the rapid development of nanoscale fabrication techniques has allowed for a significant improvement in the control over the transduction of optical signals. For example, optical nanoantennas have been used in steerable wireless links.[1] In an effort to detect the signals in optical nanoantenna links as an electrical signal, we couple nanoantenna arrays with a graphene photodetector. Such a device would act as a demonstration of tunable, on-chip, wireless transmission and detection of optical signals.

[1] Dregely, D., Lindfors, K., Lippitz, M., Engheta, N., Totzeck, M., Giessen, H., Nat. Commun., 2014, 5, 4354.

O 70.10 Wed 18:00 P2/EG

Fabrication of STM+AFM+TERS tips — •Petr Kahan, Jiří Doležal, Amandeep Sagwal, Rodrigo Ferreira, and Martin Švec — Institute of Physics, Czech Academy of Sciences; Cukrovarnická 10/112, CZ16200 Praha 6, Czech Republic

Although many highly reproducible techniques[1,2,3] exist for scanning tunneling microscopy (STM) tip preparation suitable for Tip-enhanced Raman spectroscopy (TERS), none of them was employed in noncontact atomic force microscopy (nc-AFM) relying on a lightweight tip glued to the tuning fork. Here we investigate the effects of commercially available and safe metallurgy etchants[3] on STM/nc-AFM tip fabrication from plasmonic metals[4]. We devised a simple optical apparatus for quick tip quality assessment. This allows us to see the Raman and plasmon scattering of the tip surface in various stages of preparation and determine its suitability for TERS. This might pave the way towards the first demonstration of combined STM/nc-AFM and TERS with submolecular resolution with the same tip [5] .

[1] Sasaki, S. S. et al. Rev. Sci. Instrum 84, 096109 (2013) [2] Yang, B. et al. JPCC 122, 16950-16955 (2018) [3] Walker, P. & Tarn, W. H. CRC handbook of metal etchants (CRC press, 1990) [4] Murray, W. A. & Barnes, W. L. Adv. Mater. 19, 3771-3782 (2007) [5] Xu, J. et al. Science 371 818-822 (2021)

O 71: Overview Talk Edvin Lundgren

Time: Thursday 9:30–10:15 Location: TRE Phy

Invited Talk O 71.1 Thu 9:30 TRE Phy

Surface dynamics under reaction conditions — •Edvin Lundgren — Department of Synchrotron Radiation Research, Institute of Physics, Lund university, Box 118, SE-221 00 Lund, Sweden

Catalysis is an important process and is widely applied on an industrial scale for many applications in either gas or in liquid phase. Industrial catalysts are complex materials, and consequently the gas/liquid-surface interaction between simplified single crystal surfaces and molecules in controlled environments has been studied for decades. We have in recent years explored the possibilities to perform experiments at conditions closer to those of a technical catalyst, at elevated pressures and in an electrolyte. In this contribution, recent results using in situ/operando techniques [1-5] will be presented. Armed with structural knowledge from ultra-high vacuum experiments, the dynamics of the gas or electrolyte induced structures and phases can be observed in real time. The strength and weaknesses of the experimental techniques will be discussed.

[1] S. Blomberg et al; Phys. Rev. Lett. 110 (2013) 117601.
[2] J. Gustafson et al; Science 343 (2014) 758.
[3] J. Zetterberg et al; Nat. Comm. 6 (2015) 7076.
[4] S. Pfaff et al; ACS Appl. Mater. Interfaces 13 (2021) 19530.
[5]L. Rämisch et al, Appl. Surf. Sci. 578 (2022) 152048.

O 72: Gerhard Ertl Young Investigator Award Competition

Time: Thursday 10:30–13:00 Location: CHE 89

O 72.1 Thu 10:30 CHE 89

Imaging electrons in 1D: correlated states within MoS$_2$ mirror twin boundaries — •Wouter Jolie — II. Physikalisches Institut, Universität zu Köln, Germany

Electrons are prone to strong correlations when confined into one-dimensional (1D) cavities. An ideal experimental testbed for the observation of correlated electronic behavior is found in mirror twin boundaries (MTBs) of the two-dimensional material MoS$_2$. These MTBs function as structurally perfect 1D cavities, are only weakly coupled to the environment and accessible to spatially resolved spectroscopic investigations using scanning tunneling microscopy.

In my talk I will show that the confined quasiparticles within finite MoS$_2$ MTBs transform into spin and charge modes as described by the Tomonaga Luttinger theory of strongly interacting 1D electrons [1]. In addition, a Kondo resonance, delocalized over the entire length of the MTB, emerges when the highest occupied mode is half filled [2]. The unique construction of our Kondo system enables us to directly measure the energies of both the Kondo resonance and the half filled confined level, as well as their correlated beating along the boundary. Lastly, I will outline how to alter the electronic system in MTBs through giant Fermi level shifts [3] and atomic manipulation.

[1] W. Jolie et al., Phys. Rev. X 9, 011055 (2019)
[2] C. van Efferen et al., arXiv:2210.09675 (2022)
[3] C. van Efferen et al., 2D Mater. 9, 025026 (2022)

O 72.2 Thu 11:00 CHE 89

Interface-engineered quantum states in van der Waals heterostructures — •Felix Lüpke — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Jülich, Germany

The assembly of van der Waals (vdW) materials into heterostructures enables the engineering of exotic quantum states by interface effects such as moiré and proximity. Scanning tunneling microscopy (STM) has become an important tool to study the properties of such heterostructure, because it gives direct access to the resulting structural and electronic properties. While the possibilities to combine different vdW materials in Lego-like fashion are virtually infinite, the fabrication of samples with atomically clean surfaces, as required for STM, was typically limited to air-stable or epitaxially grown samples, which drastically diminishes the engineering capabilities. To address this problem, we have developed a novel dry-transfer flip fabrication technique, which allows the preparation and STM study of heterostructures with atomically clean surfaces and interfaces and without exposure to air. In my talk, I will summarize our developments in heterostructure fabrication and will show results of proximity-induced superconductivity in topological insulator WTe$_2$, interlayer interactions in twisted bilayer WTe$_2$, phonon gap supported tunneling and interfacial electric fields in Fe$_3$GeTe$_2$ heterostructures, and quantum dot lattices in NbSe$_2$ heterostructures.

O 72.3 Thu 11:30 CHE 89

Electronic States and Polarons on Polar Surfaces — •Michele Reticcioli[1], Florian Ellinger[1], Martin Setvin[2], and Cesare Franchini[1,3] — [1]University of Vienna (Austria) — [2]Charles University, Prague (Czech Republic) — [3]University of Bologna (Italy)

Polar surfaces of oxides exhibit an internal electric field and intrinsic excess charge that might be exploited for a wide range of applications, such as catalysis or electron-hole separation for solar light harvesting. However, there is very limited fundamental understanding of the processes induced by the surface polarity. In our study we attempt to shed some light on the nature of the electric field and the interplay with surface charge. Our density functional theory calculations and scanning-probe microscopy measurements on KTaO$_3$(001) show spontaneous localization of the excess charge in the form of electron and hole polarons. In the absence of external perturbations, the internal electrostatic potential keeps the electron-hole polaron pairs spatially separated. We also show that the electronic properties of the surface can be tuned by adsorbing molecules and metal atoms. Finally, we apply these concepts to more debated cases, such as the SrTiO$_3$(001) surface, where the polarity is too weak to produce a large charge separation. We believe that our findings contribute to deepen the interpretation of polar surfaces of oxides and ionic compounds in general.

O 72.4 Thu 12:00 CHE 89

Submolecular-scale control of phototautomerization — •Anna Rosławska[1], Katharina Kaiser[1], Michelangelo Romeo[1], Fabrice Scheurer[1], Stéphane Berciaud[1], Tomáš Neuman[2], and Guillaume Schull[1] — [1]Université de Strasbourg, CNRS, IPCMS, UMR 7504, 67000 Strasbourg, France — [2]Institut des Sciences Moléculaires d'Orsay (ISMO), UMR 8214, CNRS, Université Paris-Saclay, 91405 Orsay Cedex, France.

Photochemistry plays a central role in fundamental natural and artificial reactions such as photosynthesis, photocatalysis, or phototautomerization. Here, we demonstrate that using a tunable light source focused on a scanning tunneling microscope (STM) tip we drive and control the rate of a free-base phthalocyanine (H$_2$Pc) phototautomerization with sub-molecular precision, providing a path to pilot the intrinsic reactivity of the molecule with an external controllable stimulus. In addition, we probe the excited state of the molecule, which drives the tautomerization, by recording tip-enhanced photoluminescence (TEPL) spectra and maps where varying patterns for non-resonant and resonant excitation conditions are observed. These TEPL maps reflect different atomic-scale coupling between the localized plasmonic fields and the transition dipole moment of the molecule influenced by the hydrogen switching process.

O 72.5 Thu 12:30 CHE 89

Single-molecule synthesis by scanning probe manipulation of intra- and inter-molecular reactions — •Qigang Zhong[1,2], Artur Mardyukov[2,3], Ephrath Solel[2,3], Alexander Ihle[1,2], Daniel Ebeling[1,2], Peter R. Schreiner[2,3], and André Schirmeisen[1,2] — [1]Institute of Applied Physics, Justus Liebig University Giessen (JLU), Germany — [2]Center for Materials Research, JLU, Germany — [3]Institute of Organic Chemistry, JLU, Germany

Single-molecule synthesis by scanning probe manipulation has emerged as a powerful tool not only to visualize, but also to generate and couple highly reactive molecules, which often are not accessible by traditional synthetic methods. As an example of precise "intra-molecular surgery", we demonstrate the on-surface synthesis of the structurally elusive cyclotriphosphazene (P3N3) based on STM tip-induced sextuple dechlorination of a sub-nanometer P3N3Cl6 precursor molecule on a Cu(111) surface [1]. Real-space atomic-level imaging of P3N3 reveals its planar D3h-symmetric ring structure. This method is further expanded to the inter-molecular level to construct covalent organic nanostructures molecule-by-molecule [2]. We have achieved unprecedented control over the whole reaction process including activation, lateral transfer and inter-molecular coupling of halogenated precursors on an inert NaCl surface. Our work presents strategies for synthesizing elusive molecules as well as covalent nanoarchitectures, studying structural modifications and revealing pathways of on-surface reactions.

[1] Preprint [https://doi.org/10.21203/rs.3.rs-2169632/v1]
[2] *Nature Chemistry* 13, 1133-1139 (2021)

O 73: Metal Substrates: Adsorption and Reaction of Small Molecules II

Time: Thursday 10:30–12:30 Location: CHE 91

O 73.1 Thu 10:30 CHE 91

Benchmarking machine-learned interatomic potentials for reactive surface dynamics at metal surfaces: accuracy vs speed — •Wojciech Stark[1], Julia Westermayr[1], Cas van der Oord[2], Lingjun Zhu[3], Bin Jiang[3], Gabor Csanyi[2], and Reinhard Maurer[1] — [1]University of Warwick, UK — [2]University of Cambridge, UK — [3]University of Science and Technology of China, China

Machine-learned interatomic potentials (MLIP) have become widely used tools to accelerate ab initio molecular dynamics simulations in materials science. Many promising MLIPs emerged recently, ranging from simple linear models to deep neural networks (DNN), differing in stability, accuracy, and inference time. Reactive scattering dynamics are highly sensitive to potential corrugation and low reaction probabilities require extensive ensemble averaging. Therefore, MLIPs need to combine smooth and accurate landscapes with extremely efficient inference. In this study, we compare different families of MLIPs, from atomic cluster expansion (ACE), message-passing based Neural Network SchNet and embedded atom neural networks (EANN), to equivariant neural networks such as PaiNN and MACE on the example of reactive molecular hydrogen scattering on copper. We compare these diverse methods by measuring accuracy and inference performance directly on dynamical observables. This provides a detailed picture of MLIP accuracy, speed, and learning rate that goes beyond simple train/test error analysis.

O 73.2 Thu 10:45 CHE 91

Electrooxidation of 1-cyclohexyl ethanol on Pt single crystal electrodes — •Lukáš Fusek[1,2], Maria Minichová[3], Valentín Briega-Martos[3], Lukas Fromm[1], Evanie Franz[1], Juntao Yang[1], Andreas Görling[1], Serhiy Cherevko[3], Peter Wasserchied[1,3], Olaf Brummel[1], and Jörg Libuda[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Charles University, Prague, Czech Republic — [3]Helmholtz-Institut Erlangen-Nürnberg, Germany

Isopropanol can be used as a liquid organic hydrogen carrier (LOHC), which is compatible with direct alcohol fuel cells.1 However, it has a limited hydrogen storage capacity. 1-Cyclohexyl-ethanol is a potential LOHC with an increased hydrogen storage capacity with two different functionalities, the alcohol (2 H+) and the cyclohexyl functionality (6 H+). In this study, we investigated the electrooxidation of 0.02 M 1-cyclohexyl ethanol on Pt(hkl) electrodes in 0.1 M HClO4 using cyclic voltammetry and electrochemical infrared reflection absorption spectroscopy. We demonstrate that it is possible to oxidize electrochemically 1-cyclohexyl-ethanol to acetophenone. Additionally, we observed 1-cyclohexyl-ethanone and decomposition products. The latter poison the Pt surface, limiting the electrocatalytic activity. The possibility to dehydrogenate electrochemically not only the alcohol but also the cyclohexyl functionality may enable us to increase the hydrogen storage capacity of fuel cell compatible LOHCs substantially, reaching values that are comparable to conventional LOHCs.

1.Sievi, G. et al. Energy Environ Sci 12, 2305-2314 (2019).

O 73.3 Thu 11:00 CHE 91

Ab initio-based chemisorption and thermodynamic stability of atomic H and O on Pt-Ir alloy surfaces — •Tobias Wittemann, Thorsten Klüner, and Halil Ibrahim Sözen — Institute of Chemistry, Carl-von-Ossietzky University of Oldenburg, 26129 Oldenburg, Germany

Electric vehicles powered by proton-exchange membrane (PEM) fuel cells are a CO_2 emission-free alternative to conventional fossil fuel vehicles. In this study, we report density functional theory (DFT) investigations of binary Pt-Ir surfaces, which are a promising candidate for bifunctional anode catalysts in PEM fuel cells that could enable higher long-term durability of the anode catalyst. The chemisorption behaviour of atomic H and O on bimetallic $Pt_3Ir(111)$ and PtIr(111) surfaces was investigated for different coverages and compared with the monometallic Pt(111) and Ir(111) surfaces. We found that in both cases the chemisorption on the alloys becomes more stable with increasing number of Ir atoms at the adsorption site. Using the *ab initio* thermodynamics approach, we calculated phase diagrams for the chemisorption of atomic H and O species on these metal surfaces in order to transfer our findings to finite temperature and pressure conditions prevailing in real PEMFCs. Our theoretical results can provide a fundamental understanding for subsequent studies of the hydrogen oxidation reaction (HOR) and oxygen evolution reaction (OER) on Pt-Ir alloy surfaces and are thus crucial for the rational development of new anode catalyst materials.

O 73.4 Thu 11:15 CHE 91

Approaching electrochemical interfaces by computational spectroscopy — •Holger Euchner[1], Jongmin Kim[1,2], Margot Guidat[1], Mario Löw[2], and Matthias M. May[1,2] — [1]Institute of Physical and Theoretical Chemistry, Universität Tübingen, 72076 Tübingen, Germany — [2]Institute of Theoretical Chemistry, Universität Ulm, 89081 Ulm, Germany

Understanding interfacial processes on the atomistic scale is essential for improving and tailoring the performance of electrochemical devices. Unfortunately, due to limited experimental access to the electrochemical interface such understanding is difficult to obtain. Applying reflection anisotropy spectroscopy (RAS), an operando optical high resolution technique, to electrochemical interfaces can help to overcome this issue. However, the information contained in experimental RAS spectra needs to be interpreted by comparison with those of computational model systems. In this work, we present computationally determined spectra for different metal electrode surfaces and analyze the impact of adsorbants on the resulting RAS signal. For this purpose, the surface dielectric function is determined by applying the random phase approximation. Finally, the obtained spectra are compared to available experimental data, showing the potential power of this approach.

O 73.5 Thu 11:30 CHE 91

Atomistic Insights at Au(111) / Deep Eutectic Solvents Interface using in situ STM — •Yannick Mattausch[1], Areeg Abdelrahman[1], Maren-Kathrin Heubach[1], Ludwig A. Kibler[1], and Timo Jacob[1,2,3] — [1]Institute of Electrochemistry, Ulm University, Ulm, Germany. — [2]Helmholtz-Institute-Ulm (HIU), Ulm, Germany. — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany.

Deep eutectic solvents (DESs) have outstanding electrochemical characteristics such as high electrochemical stability and conductivity.[1][2] Nonetheless, the interactions between the metal electrode surface and DESs besides their electrochemical behavior, like the electrolyte / Au(111) interface structure are still poorly understood. Recently, the electrochemical behavior and adsorption structures of Au(111) in Ethylenglycole / Cholinchloride (2:1) have been studied, including an ordered chloride structure at 0.1 V *vs.* Pt and the potential induced surface reconstruction of Au(111).[3] Here, we go a step further by changing the electrolyte composition and studying its influence on the electrochemical behavior as well as the dynamics at the electrode-electrolyte interface at an atomistic level. To reach this aim, *in situ* scanning tunneling microscopy (STM) is employed to observe morphological changes at the electrode surface in real time and space.

[1] Smith, E. L., Abbott, A. P. Ryder, K. S., *Chem. Rev.* **114**, 11060–11082 (2014). [2] Abbott, A. P., D'Agostino, C., Davis, S. J., Gladden, L. F. Mantle, M. D. *Chem. Chem. Phys.* **18**, 25528–25537 (2016). [3] Tan, Z. *et al.*, *ChemElectroChem* **7**, 4601–4605 (2020).

O 73.6 Thu 11:45 CHE 91

2D chiral crystallization and thermally-induced on-surface polymerization of 2,3-dicarbonitrile-tetrahelicene on Ag(111) surface — •Aleksandra Cebrat[1,3], Christian Wäckerlin[1], Kevin Martin[2], Manfred Parschau[1], Narcis Avarvari[2], and Karl-Heinz Ernst[1,3] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland — [2]Laboratoire Moltech-Anjou, CNRS-Université d'Angers, 49045 Angers, France — [3]Department of Chemistry, University of Zurich, 8057 Zürich, Switzerland

The controlled on-surface polymerization using templates like metal surface and non-planar molecules can lead to synthesis of variable phthalocyanines and organic semiconducting polycyanine open-chains. Here, we report the initial results on the 2D chiral crystallization of racemic mixture of 2,3-dicarbonitrile-tetrahelicene on Ag(111) and its thermally-induced surface polymerization. Deposition of racemic diCN[4]H up to 0.9ML coverage on Ag(111) kept at 300 K leads to formation of islands of honeycomb domains built of M- and P-enantiomers. Deposition of rac-diCN[4]H on 330K up to 0.9ML leads to aggregation of molecules into long molecular lines and denser phase of unbalanced domains with either enantiomers present in excess. Subsequent annealing to 420 K leads to partial desorption of molecular lines and formation of single tetramers built from different stereoisomeric subunits. The formation of polymerized species was confirmed ToF-SIMS. Finally, we performed LT-STM lateral manipulation of the tetramers units to affirm the nature of bonds as covalent.

O 73.7 Thu 12:00 CHE 91

Interaction of chlorine with lithium and magnesium anodes in Cl-ion batteries — •Kanchan Sarkar[1] and Axel Gross[1,2] — [1]Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany — [2]Helmholtz Institute Ulm (HIU), Electrochemical Energy Storage, 89069 Ulm, Germany

We present the results of first-principles electronic structure calculations based on density functional theory addressing the adsorption of chlorine and the formation of a surface chloride on Li(001) and Mg(0001). This process is relevant for chloride-ion batteries in which lithium and magnesium are used as anode materials, but it is also of fundamental interest, as halide adsorption on metal electrodes is an important process in electrochemistry. We discuss the adsorption properties and determine the stable adsorption structures, both with respect to the free chlorine molecule but also as a function of the electrode potential. We will also address the process of chloride formation on the surface.

O 73.8 Thu 12:15 CHE 91

Bromine on Rh(111) - A combined XPS and LEED study — •Eva Marie Freiberger[1], Natalie J. Waleska[1], Anton Harrer[1], Felix Hemauer[1], Valentin Schwaab[1], Hans-Peter Steinrück[1], and Christian Papp[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Freie Universität Berlin, Berlin, Germany

The adsorption of halogens on metals is a fundamental question in surface science. Detailed knowledge in this regard is of interest for any processes on surfaces, in which halogens are involved as a reactant or by-product. This plays a role, for example, in electrochemistry, when the electrolyte adsorbs at the electrodes, or in on-surface synthesis, which often relies on coupling reactions with halogens as the leaving group, leading to their accumulation on the surface.

We investigated the adsorption and thermal evolution of elemental bromine on the Rh(111) single-crystal surface by synchrotron radiation-based high-resolution X-ray photoelectron spectroscopy (XPS), temperature-programmed XPS, and low energy electron diffraction (LEED). The adsorption of bromine on Rh(111) held at 170 K was followed in situ by XPS, revealing a coverage-dependent shift in the Br 3d spectra. Using LEED as a complementary method, we propose that the observed shift is caused by different bromine superstructures on Rh(111): a $(\sqrt{3}\ \mathrm{x}\ \sqrt{3})$R30° structure for lower coverages and a compression structure for saturation coverage. Subsequent heating shows a quite high temperature stability of bromine on Rh(111) up to 925 K, indicating covalent bonding.

O 74: 2D Materials IV: Heterostructures (joint session O/CPP)

Time: Thursday 10:30–12:45 Location: GER 37

O 74.1 Thu 10:30 GER 37

In-situ growth characterization of 2D heterostructures: MoSe$_2$ on intercalated graphene/Ru(0001) — •Lars Buss[1], Nicolas Braud[2], Moritz Ewert[1], Matteo Jugovac[3], Tevfik Onur Mentes[3], Andrea Locatelli[3], 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 — [3]Elettra-Sincrotrone Trieste S.C.p.A, Bazovizza, Trieste, Italy

Despite the great fundamental interest in 2D heterostructures, most of the investigated 2D heterostructures were realized by mechanical exfoliation or chemical vapor deposition in the millibar range, preventing true in-situ characterization of the growth process. Here, we have investigated the growth of MoSe$_2$ on single-layer graphene on Ru(0001) via real-time in-situ low-energy electron microscopy and micro-diffraction. After preparation of the graphene by standard procedures from an ethylene precursor, MoSe$_2$ has been prepared via codeposition of Mo and Se. Prior Se intercalation of the graphene appears to enhance the subsequent growth of MoSe$_2$ on the graphene. At elevated temperatures, rotational ordering of the MoSe$_2$ is facilitated by the strongly enhanced mobility of single-domain MoSe$_2$ islands that align with the high symmetry orientations of the underlying graphene, indicating a non-negligible interaction between the two van-der-Waals materials. Micro-spot angle-resolved photoemission proves the monolayer nature of the as-grown MoSe$_2$ as well as the free-standing character of the Se-intercalated graphene underneath.

O 74.2 Thu 10:45 GER 37

Designer quantum states in metal-organic frameworks — •Orlando J Silveira[1], Linghao Yan[1], Shawulienu Kezilebieke[2], Benjamin Alldritt[1], Viliam Vano[1], Ondřej Krejčí[1], Jose Lado[1], Adam S Foster[1,3], and Peter Liljeroth[1] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]University of Jyväskylä, FI-40014 University of Jyväskylä, Finland — [3]Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Vertical heterostructures have emerged as a promising path to the design of quantum materials with exotic properties. Here, we show that this concept can be also extended to a family of 2D kagome metal-organic frameworks (MOFs) of the family M$_2$DCA$_3$, with M= Cu and Ni. The two MOFs have been fabricated either on a graphene/Ir(111) surface or the superconducting substrate NbSe$_2$, and the structural and electronic properties of different phases of both 2D MOFs + substrates were studied through density functional theory (DFT) calculations. Results show that the Cu$_2$DCA$_3$ MOF is effectively decoupled from the Ir(111) metallic substrate by the graphene layer, which is important to reveal the topological properties of this family of MOF. Moreover, this study extends the synthesis and electronic tunability of 2D MOFs beyond the metal surfaces to superconducting substrates, which are needed for the development of emerging quantum materials. We show that the Ni$_3$DCA$_2$ MOF has a spin density around the Ni atom when synthesized on the NbSe$_2$ substrate due to charge transfer, and this makes a perfect platform to realize topological superconductivity.

O 74.3 Thu 11:00 GER 37

Phonon gap supported tunneling and Faraday screening through graphene — •Tobias Wichmann[1,2,3], Keda Jin[1,2,4], Jose Martinez Castro[1,4], Honey Boban[5], Lukasz Plucinski[5], Markus Ternes[1,2,4], F. Stefan Tautz[1,2,3], and Felix Lüpke[1,2] — [1]Peter-Grünberg-Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - 52425 Jülich, Fundamentals of Future Information Technology, Germany — [3]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany — [4]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany — [5]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany

Encapsulation of van der Waals materials has proven a vital technique to protect them from degradation and contamination. Usually, metallic encapsulation layers mask the properties of the underlying material when studied in scanning tunneling microscopy. Utilizing the inelastic tunneling phonon gap of graphene, however, enables the unfettered investigation of low energy phenomena (e.g. Kondo effect, Majoranas, etc.) by scanning tunneling spectroscopy, while maintaining the advantages of encapsulated samples. Furthermore, we find that the conductive nature of the graphene encapsulation layer screens the sample from tip-induced electric fields, exemplified by our low-temperature STM examination of encapsulated Fe3GeTe2.

O 74.4 Thu 11:15 GER 37

Fermi level tuning of a MnBi$_2$Te$_4$ monolayer — •Marco Dittmar[1], Philipp Kagerer[1], Celso I. Fornari[1], Simon Müller[1], Sergio L. Morelhão[2], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — [2]Instituto de Física, Universidade de São Paulo, Brazil

By breaking time reversal symmetry, introducing magnetic order to topological insulators leads to the opening of a 2D surface state gap at the Dirac point. As a second crucial parameter, tuning the position of the Fermi level inside this gap, enables the observation of exciting new phenomena, such as the quantum anomalous Hall effect (QAHE). Here, we focus on the intrinsic ferromagnetic monolayer of MnBi$_2$Te$_4$, acting as a magnetic extension of the topological insulator Bi$_2$Te$_3$ [1]. We tune the Fermi level position in this compound by preparing a single layer of MnBi$_2$Te$_4$ on top of the topologically non-trivial p-n-junction of Sb$_2$Te$_3$ and Bi$_2$Te$_3$ grown by molecular beam epitaxy (MBE) [2]. We will present a study containing structural characterization of the heterostructures by X-ray diffraction and atomic force microscopy, while the electronic structure is assessed by X-ray and angle resolved photoemission spectroscopy.

[1] M. M. Otrokov *et al.*, 2D Mater **4**, 025082 (2017)
[2] P. Kagerer *et al.*, arXiv 2207.14421 (2022)

O 74.5 Thu 11:30 GER 37

1D Topological Superconductivity in a van der Waals heterostructure probed by Abrikosov vortices — •Jose Martinez-Castro[1,2], Tobias Wichmann[1,3], Tomáš Samuely[4], Keda Jin[1,2], Oleksander Onufriienko[4], F. Stefan Tautz[1,3,5], Markus Ternes[1,2,3], and Felix Lüpke[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany. — [3]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, 52425 Jülich, Germany — [4]Centre of Low Temperature Physics, Faculty of Science, P. J. Safarik University & Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia — [5]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany

The 2D topological insulator monolayer (ML) WTe$_2$ is characterized by an insulating interior surrounded by helical 1D edge states. When this material is brought into proximity to the s-wave superconductor NbSe$_2$, the spectroscopic features of the helical edge state remain intact while showing a proximity-induced superconducting gap [1]. However, so far there has been no direct evidence that the observed edge superconductivity is of different nature than that observed away from the edge. Here, by inducing Abrikosov vortices at the boundary between ML WTe$_2$ and NbSe$_2$, we show that the induced superconductivity in the helical edge is robust against magnetic fields, a strong indication of 1D topological superconductivity.

[1] Lüpke et al., Nat. Phys. 16, 526 (2020)

O 74.6 Thu 11:45 GER 37

Density functional theory studies of Anthracene on MoS$_2$ — •Gérald Kämmerer and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen

Thin layers of MoS$_2$ are attractive as transparent contacts on organic semiconductors, e.g., oligoacene. As a model for molecules with a delocalized system of π-bonds, we investigate the physisorption of a monolayer of anthracene ($C_{14}H_{10}$) on a MoS$_2$ single layer using density functional theory. The calculations were carried out with the FHI-Aims code with different functionals. Van der Waals interactions are described by a pairwise potential of the Tkatchenko-Scheffler type or by a many-body dispersion technique. We determine structural properties and can identify the relative position of the molecular HOMO and LUMO (Π and Π^*) orbital concerning the band edges of MoS$_2$. These results can help find the type of band alignment between MoS$_2$ and an anthracene molecular crystal, as well as the binding energy of the molecule on the surface. The financial support by DFG within CRC 1242 (*Project B 02*) and computation time on the MagnitUDE supercomputer system are gratefully acknowledged.

O 74.7 Thu 12:00 GER 37

Lateral heterostructures of graphene and h-BN with atomic lattice coherence and tunable rotational order — •Haojie Guo[1], Ane Garro-Hernandorena[1], Antonio J. Martínez-Galera[2,3], and José M. Gómez-Rodríguez[1,3,4] — [1]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [4]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

In-plane heterostructures of graphene and h-BN exhibit exceptional properties, which are sensitive to the structure of the alternating domains. However, achieving accurate control over their structural properties, while keeping a high perfection of the graphene-h-BN boundaries, still remains a challenge. Here, the growth of lateral heterostructures of graphene and h-BN on Rh(110) surfaces is reported. The choice of the 2D material, grown firstly, determines the structural properties of the whole heterostructure layer, allowing to have control over the rotational order of the domains. The atomic-scale observation of the boundaries demonstrates a perfect lateral matching. Lateral heterostructures floating over an oxygen layer have been successfully obtained, enabling to observe intervalley scattering processes in graphene regions. The high tuning capabilities of these heterostructures suggests their usage as testbeds for fundamental studies.

O 74.8 Thu 12:15 GER 37

Relaxation mechanisms for in-plane heterostructures of transition metal dichalcogenide monolayers — •Kai Mehlich[1], Francis H. Davis[3], Thais Chagas[1], Daniela Dombrowski[2], Daniel Weber[1], Catherine Grover[1], Arkady Krasheninnikov[3], and Carsten Busse[1] — [1]Derpartment Physik, Universität Siegen, Walter-Flex-Str. 3, 57072 Siegen — [2]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [3]Ion Beam Centre, Helmoltz-Zentrum Dresden Rossendorf, Bautzner Landstraße 400, 01328 Dresden

We use sequential epitaxial growth to synthesise in-plane heterostructures of MoS$_2$ and TaS$_2$ monolayers on Au(111). Even though the two materials have significantly different lattice constants, STM-measurements show that coherent interconnection of the two materials can be achieved. Defects at the interface such as dislocations are absent. We find this for all interfaces, independent of orientation or the widths of the joined materials. This is at variance with DFT-calculations where we find that the formation of dislocations is energetically favoured, at least until a critical width of the heterostructures. Our growth process can thus lead to a metastable, defect-free interface.

O 74.9 Thu 12:30 GER 37

Predicting the Gas Sensing Performance of 2D Materials — •Udo Schwingenschlögl, Vasudeo Babar, Hakkim Vovusha, and Altynbek Murat — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

We study the potential of material simulations based on first-principles methods to predict gas sensing properties of 2D materials. This emerging class of materials is of particular interest to gas sensing applications due to high surface-to-volume ratios and chemical stability. We discuss results of electron transport calculations within the Landauer-Büttiker formalism and compare the conclusions to analyses in terms of the adsorption energy. Journal References: ACS Appl. Nano Mater. 2, 6076 (2019); J. Phys. Condens. Matter 32, 355602 (2020)

O 75: Focus Session: Ultrafast Dynamics in Nanostructures I

In nanostructures, the response of electrons and atoms to external stimuli often differs significantly from that of their bulk counterparts due to spatial confinement and greatly increased surface-to-volume ratios. Whereas pump-probe techniques provide real time access to the dynamics of nanostructures in excited states, investigating the response of single nanostructures and probing their dynamics locally requires ultrafast imaging techniques that provide simultaneously a high spatial and temporal resolution.

Several ultrafast nanoscale imaging methodologies have made a tremendous progress in recent years. Crucial instrumental developments have enabled time-resolved variants of scanning probe techniques, such as ultrafast scanning near-field optical microscopy and ultrafast scanning tunneling microscopy. Furthermore, bright sources for femtosecond electron as well as extreme ultraviolet and x-ray pulses now allow for the ultrafast far-field probing with nanometer resolution.

To highlight these recent developments, this focus session brings together researchers interested in ultrafast nanoscale science and in the development of ultrafast high-resolution imaging approaches.

Organizers: Melanie Müller (FHI Berlin) and Sascha Schäfer (U Regensburg)

Time: Thursday 10:30–13:15 Location: GER 38

Topical Talk O 75.1 Thu 10:30 GER 38

Ultrafast nano-imaging: probing quantum dynamics in space and time — •Markus Raschke — Department of Physics and JILA, University of Colorado, Boulder, USA

Understanding and ultimately controlling the properties of matter, from molecular to quantum systems, requires imaging the elementary excitations on their natural time and length scales. To achieve this goal, we developed scanning probe microscopy with ultrafast and shaped laser pulse excitation for multiscale spatio-temporal optical nano-imaging. In corresponding ultrafast movies we resolve the fundamental quantum dynamics from the few-femtosecond coherent to the thermal transport regime. I will discuss specific examples visualizing in space and time the nanoscale heterogeneity in competing structural and electronic dynamic processes that define the performance in perovskite photovoltaics or energy dissipation in 2D heterostructures. I will extend the discussion to new forms of photon-matter hybrid states that emerge from confining light on the nano- to atomic scale, with imaging in tip-enhanced strong coupling of single emitters, to new regimes of nonlocal and quantum nonlinear nano-optics.

O 75.2 Thu 11:00 GER 38

Towards a nanoscale ultrafast optical oscilloscope — •Abbas Chimeh, Sam Nochowitz, Tom Jehle, Juanmei Duan, Sven Stephan, and Christoph Lienau — Universität Oldenburg

Measuring the ultrafast time response on the nanoscale gives insights into the complex structure and dynamics of nanomaterials. A variety of all-optical and electron-based spectroscopy techniques are currently under development to probe such ultrafast dynamics [1].

Here, we propose and demonstrate a broadband, interferometric scattering-type scanning near-field optical spectroscopy technique to measure ultrafast response function on the nanoscale. The idea is to mix the weak optical near field that is scattered out from the gap of a laser-illuminated tip-sample junction with a broadband reference pulse in a single spatial mode. From the resulting phase-stable spectral interferogram, we can directly retrieve the linear optical response function of the coupled tip-sample system and, thus, the time structure of re-emitted electric field with sub-cycle precision. By recording scattering spectra at a rate much higher than typical tip-sample modulation frequencies, we can separate the near-field response from unmodulated signal backgrounds and directly probe the time structure of optical near-fields on the nanoscale. We demonstrate the technique by probing local light scattering from single TMDC monolayers. Our technique provides a general approach for measuring the response functions of nanostructures in the visible and near-infrared spectral range with femtosecond temporal and nanometer spatial resolution.

[1] P. Dombi et al., Rev. Mod. Phys., 92, 025003 (2020).

O 75.3 Thu 11:15 GER 38

Ultrafast electron dynamics in semiconductor nanowires — •Jan Vogelsang[1,2], Lukas Wittenbecher[1], Cord L. Arnold[1], Anne L'Huillier[1], and Anders Mikkelsen[1] — [1]Department of Physics, Lund University, 221 00 Lund, Sweden — [2]present address: Institut für Physik, Universität Oldenburg, 26129 Oldenburg, Germany

The dynamics and, in particular, the transport of charge carriers in semiconductor nanostructures after optical excitation are influenced by different processes whose interaction is not yet fully understood. Here, we employ ultrashort laser pulses in combination with a photoemission electron microscope (PEEM) to spatiotemporally resolve these processes. We observe the radial transport of charge carriers in semiconductor nanowires after impulsive optical excitation and investigate the influence of electron-hole scattering on the relaxation times of hot electrons. We conclude with a glimpse on an attosecond streaking experiment in a PEEM promising an even higher temporal resolution.

O 75.4 Thu 11:30 GER 38

SPP induced coherent electronic excitations investigated by Time- and Angle-Resolved Plasmoemission-Spectroscopy on Cs/Au(111) — •Alexander Neuhaus, Pascal Dreher, David Janoschka, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany

Non-perturbative interactions of intense light fields with the electronic band structure in a solid can result in transient electronic properties. The experimental conditions required to realize the necessary field strength can be realized in nano-optical systems, as these can be designed to provide tremendous enhancements of the local field amplitude. Ultimately, observing the non-equilibrium electron dynamics in such systems requires a combination of precise control over the local driving field, state resolution, and spatial selectivity. Here, we explore electron emission from nano-focused femtosecond surface plasmon polariton (SPP) pulses, providing us with deep-subwavelength spatial selectivity. Two-dimensional time- and angle-resolved photoelectron spectroscopy using a birefringent delay line provides us with direct access to the coherent and incoherent dynamics of the electronic excitations with attosecond precision. The technique is applied to the system Cs/Au(111), where we observe SPP induced coherent electronic excitations of the first image potential state.

Topical Talk O 75.5 Thu 11:45 GER 38

Lightwave-driven scanning tunneling microscopy and spectroscopy at the atomic scale — •Vedran Jelic[1], Spencer E. Ammerman[1], Yajing Wei[1], Vivian N. Breslin[1], Mohammed Hassan[1], Nathan Everett[1], Sheng Lee[1], Stephanie Adams[1], Trevor Hickle[1], Kaedon Cleland-Host[1], Qiang Sun[2], Carlo A. Pignedoli[2], Pascal Ruffieux[2], Roman Fasel[2,3], and Tyler L. Cocker[1] — [1]Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA — [2]Empa Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — [3]Department of Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern, 3012 Bern, Switzerland

Lightwave-driven scanning tunneling microscopy is a new technique for studying atomic-scale surfaces that exhibit sub-picosecond dynamics. By coupling free-space-propagating single-cycle terahertz pulses to an atomically sharp metal tip, lightwave-driven microscopy can achieve simultaneous sub-angstrom and sub-picosecond spatio-temporal resolution. We utilize terahertz scanning tunneling microscopy (THz-STM) to investigate seven-atom-wide graphene nanoribbons on an Au(111) surface and unveil highly localized wavefunctions that are inaccessible with conventional STM. Three-dimensional tomographic THz-STM imaging of the electron densities reveals a faster spatial decay of the valance band compared to the conduction band. Additionally, an algorithm is introduced for extracting the underlying differential conductance from THz-STS measurements in both steady-state and pump-probe scenarios.

O 75.6 Thu 12:15 GER 38

Probing hot electron dynamics in a metal nanotip with THz-STM — •Vivien Sleziona[1], Faruk Krecinic[1], Natalia Martín Sabanés[1,2], Fabian Schulz[1,3], Takashi Kumagai[1,4], Martin Wolf[1], and Melanie Müller[1] — [1]Fritz-Haber Institute, Berlin — [2]IMDEA Nanoscience, 28049 Madrid, Spain — [3]CIC NanoGUNE, San Sebastian, Spain — [4]Institute of Molecular Science, 444-8585 Okazaki, Japan

In metal nanostructures, such as the tip of a scanning tunneling microscope (STM), the excitation and dynamics of hot electrons can differ significantly from their behavior in bulk solids. However, how exactly the electrons in an STM tip respond to femtosecond (fs) laser excitation is still poorly understood, although this is important for optimizing and understanding fs-laser-excited STM operation. Here we use a THz-gated STM to study the ultrafast dynamics of photoexcited electrons in a tungsten STM tip [1]. Specifically, we investigate the role of thermalized hot electrons for the generation of ultrafast photocurrents and tunneling in STM. Knowledge of the THz voltage transient combined with simulation of the electron dynamics inside the confined volume of the STM tip allows us to extract the electronic temperature and its ultrafast decay. We evaluate the relevance for fs laser-excited STM and discuss how the tip geometry affects electronic heating on ultrafast time scales. [1] N. Martín Sabanés et al., ACS Nano 16, 9, 14479-14489 (2022)

O 75.7 Thu 12:30 GER 38

Spin current control by hybrid pulses — •Jyoti Krishna[1], Sangeeta Sharma[2], Julen Ibañez-Azpiroz[1,3], and Sam Shallcross[2] — [1]Centro de Fisica de Materiales (CSIC-UPV/EHU), 20018, San Sebastian, Spain — [2]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max-Born-Straße 2A,12489 Berlin — [3]Ikerbasque Foundation, 48013 Bilbao, Spain

Spin and valley indices represent the key quantum labels of quasiparticles in a wide class of two dimensional materials, and control over these degrees of freedom, the creation of valley and spin states as well as the generation of pure spin and valley currents, remains a central challenge in these fields. Here we show that hybrid femtoscond laser pulses combining optical frequency circularly polarized pulse and a terahertz frequency linearly polarized pulse, a so-called "hencomb" pulse, can generate currents, whose magnitude and direction can be precisely controlled by the THz envelope. We explore this effect both in bilayer graphene and the dichalocogenide WSe_2, finding control over substantial currents that are nearly 100% pure valley and spin currents respectively. Employing a Wannier tight-binding method we then explore the creation of coherent photocurrents in the 2d magnets CrI_3 and FGT, generalizing the role of the THz and optical pulses to "momentum guiding" and "excitation" components of hybrid laser pulses.

Funding was provided by the European Union's Horizon 2020 research and innovation programme under the European Research Council (ERC) grant agreement No 946629.

O 75.8 Thu 12:45 GER 38

Mode-selective ballistic pathway to a metastable electronic phase — •Hannes Böckmann[1,2], Jan Gerrit Horstmann[3], Felix Kurtz[1,2], Abdus Samad Razzaq[4], Stefan Wippermann[4], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen 37077, Germany — [2]4th Physical Institute, Solids and Nanostructures, University of Göttingen — [3]Department of Materials, ETH Zurich, Zurich — [4]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Exploiting vibrational excitation for the dynamic control of material properties is an attractive goal with wide-ranging technological potential. Most metal-to-insulator transitions are mediated by few structural modes and are, thus, ideal candidates for selective driving toward a desired electronic phase. Such targeted navigation within a generally multi-dimensional potential energy landscape requires microscopic insight into the non-equilibrium pathway. However, the exact role of coherent inertial motion across the transition state has remained elusive. Here, we demonstrate mode-selective control over the metal-to-insulator phase transition of atomic indium wires on the Si(111) surface, monitored by ultrafast low-energy electron diffraction. We use tailored pulse sequences and spectrally selective excitation to individually enhance or suppress key phonon modes and thereby steer the collective atomic motion within the potential energy surface underlying the structural transformation. Our work illustrates that coherent excitation of collective modes via exciton-phonon interactions evades entropic barriers and enables the dynamic control of functionality.

O 75.9 Thu 13:00 GER 38

Nanoscale coherent phonon excitation via plasmon-matter interaction in ultrathin ZnO films — •H. Wiedenhaupt[1], S. Liu[1,2], L. Parra López[1], A. Hammud[1], I. Hamada[3], F. Schulz[1,4], M. Wolf[1], T. Kumagai[1,2], and M. Müller[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]Institute for Molecular Science, Okazaki 444-8585, Japan — [3]Hunan University, Hunan 410082, P. R. China — [4]CIC NanoGUNE, San Sebastian, Spain

In crystalline nanostructures, nanoscale variations of the lattice and/or electronic structure can alter their microscopic response and its interaction with light. Using light-coupled scanning tunneling microscopy (STM) with plasmonic junctions, we demonstrated recently that the local electronic structure of ultrathin ZnO on Ag(111) can strongly affect light-matter interaction on the nanoscale. Specifically, resonant laser excitation of these films seems crucial for tip-enhanced Raman spectroscopy (TERS) [1] and for the nanoscale excitation and observation of coherent phonon dynamics [2]. CPs are excited by femtosecond excitation of localized surface plasmons (LSP), and modulate the femtosecond photocurrent in the STM on ultrafast time scales. To better understand the optical excitation mechanism in these films, we measure plasmon-enhanced STM-induced luminescence, which allows us to correlate the local electronic structure of the films with their light coupling efficiency on the nanoscale. [1] S. Liu, Nano Lett. 19, 5725 (2019), [2] S. Liu et al., Sci. Adv. 8, eabq5682 (2022)

O 76: Plasmonics and Nanooptics III: Light-Matter Interaction and Spectroscopy II

Time: Thursday 10:30–12:45 Location: WIL A317

O 76.1 Thu 10:30 WIL A317

Continuous-wave multiphoton-induced electron transfer in a biased tunnel junction driven by intense plasmonic fields — Chenfang Lin[1], •Melanie Müller[1,2], Faruk Krecinic[1], Hiroko Yoshino[1], Adnan Hammud[1], Anlian Pan[2], Martin Wolf[1], and Takashi Kumagai[3] — [1]Fritz Haber Institute, Faradayweg 4-6, Berlin — [2]Hunan University, Hunan 410082, China — [3]Institute for Molecular Science, Okazaki 444-8585, Japan

Understanding photoinduced tunneling processes in the presence of intense plasmonic fields is of crucial importance for the design of plasmon-induced hot carrier technology and optical rectennas. However, in contrast to femtosecond laser excitation, the observation of multiphoton-induced electron transfer and the understanding of the role of hot carriers under intense continuous-wave (cw) illumination remains scarce. Here we exploit the strong spatial confinement of light inside the plasmonic gap of a scanning tunneling microscope (STM) to drive photocurrents with cw optical fields at local peak intensities up to 10^9 W/cm^2 at low incident power. We find that the photoinduced tunneling current scales nonlinear (linear) with laser intensity at low (high) STM bias. To yield insight into the photoinduced tunneling process we analyze the photocurrent-voltage dependence for different laser wavelength and powers. We discuss two possible origins of the multiphoton-induced electron transfer, namely transport of photoexcited hot electrons and photon-assisted quantum tunneling into light-dressed states.

O 76.2 Thu 10:45 WIL A317

Atomically resolved optical spectroscopy and microscopy in a scanning-tunneling microscope: Theory and experiment — •Tomas Neuman[1,2], Anna Roslawska[1], Benjamin Doppagne[1], Andrei G. Borissov[2], Michelangelo Romeo[1], Fabrice Scheurer[1], Javier Aizpurua[3], and Guillaume Schull[1] — [1]Universite de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000, Strasbourg, France — [2]Institut des sciences Moleculaires d'Orsey (ISMO), UMR 8214, CNRS, Universite Paris-Saclay, 91405 Orsay Cedex, France — [3]Center for Materials Physics and DIPC, Paseo Manuel de Lardizabal 5, Donostia-San Sebastian 20018, Spain

We present a joint theoretical and experimental study of the optical properties of individual small organic molecules excited electrically by the plasmonic tip of a STM. We investigate how these properties vary as a function of the tip position with atomic-scale resolution. We show that the variation of the spectral position and width of the electroluminescence emission line of the molecular exciton can be linked with the DC Stark effect (induced by the static voltage across the tip-substrate gap) and the plasmonic Purcell effect due to the plasmonic response of the tip, respectively. We interpret the spectral line shift map as an image of the difference between the excited- and ground-state electron densities of the molecule, and the tip-position-dependent map of the excitonic line-width variation as an image of the transition electron density. In contrast, the map of light intensity emitted by the molecule reveals the information about the electronic mechanism leading to the tip-mediated generation of the exciton.

O 76.3 Thu 11:00 WIL A317

Modeling of molecular systems probed by near-field spectroscopy — •Sofia Canola, Jiří Doležal, Rodrigo Ferreira, and Martin Švec — Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic

Spectroscopy coupled to scanning-probe microscopy is a powerful tool to analyze molecular properties at a single molecule level with submolecular resolution. In this technique, some intrinsic limitations and selection rules of conventional spectroscopy are overcome. This aspect, together with the high resolution of the signal and the precise control over the sample, allow to obtain information otherwise not accessible, such as for example the structural arrangement of the molecule, the electronic structure of its ground or excited molecular electronic state, its charging state or its response to stimuli. To fully unpack and rationalize the information, a theoretical interpretative framework must accompany the experimental findings. A crucial aspect is the ability to describe the molecular spectroscopic response in the near-field while including all the relevant aspects of the setup. High-level quantum-chemical calculations are needed, capable of reliably modeling the molecular system in its complexity and providing the appropriate response function. In this contribution, we present the results from the application of this technique to small conjugated molecules, with particular focus on the modeling aspects and the interesting molecular properties that become accessible when experiments and theory complement.

O 76.4 Thu 11:15 WIL A317

Plasmon-Induced Molecular Switching of PTCDA on Si(111) Studied by STM-TERS — •Youngwook Park[1], Adnan Hammud[1], Martin Wolf[1], Takashi Kumagai[2], and Akitoshi Shiotari[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Institute for Molecular Science, Okazaki, Japan

We studied a unique plasmon-induced molecular motion of perylenetetracarboxylic dianhydride (PTCDA) single molecules on the Si(111)-7x7 surface by means of the atomic point contact (APC) tip-enhanced Raman spectroscopy (TERS) with a low temperature scanning tunneling microscope (STM) under an ultrahigh vacuum condition. In our APC-TERS scheme, a silver tip approaches close to the surface until the tip makes an atomic point contact with its counterpart. It was reported by our previous study that at the point contact with Si(111) the TERS signal was significantly enhanced. The PTCDA on the Si(111), fixed on the surface by four oxygen-silicon bonds, showed a distinctive APC-TERS pattern where the Raman intensity was dramatically enhanced at a certain gap distance during the tip approach, and then was attenuated at shorter tip-molecule distances. At the TERS "sweet spot", the STM current rapidly switched between two states, implying a fluctuative motion of PTCDA molecule between the tip and the surface. On the contrary to PTCDA, perylenetetracarboxylic diimide (PTCDI) did not show such TERS "sweet spot" nor STM current switching. We believe this unique system could provide a better understanding on the plasmon-molecule interaction, as well as their implication on the enhancement mechanism in TERS.

O 76.5 Thu 11:30 WIL A317

Photoluminescence mapping of an anionic molecule — •Jiří Doležal, Rodrigo Ferreira, Amandeep Sagwal, Petr Kahan, and Martin Švec — Institute of Physics, Czech Academy of Sciences; Cukrovarnická 10/112, CZ16200 Praha 6, Czech Republic

Only recently, the photoluminescence (PL) of a single molecule has been attained [1,2] with sub-nm resolution in a scanning tunneling microscope (STM). However, only a fluorescent peak from a neutral phthalocyanine has been observed. The observation of fluorescence from a charged molecule is still elusive, likely due to the plasmon-mediated excitation mechanism which is fundamentally different from the electroluminescence (EL) process where a charged exciton can be created via electron/hole tunneling into dication/dianion [3,4].

Here, we present STM-PL maps of PTCDA anion adsorbed on 3ML/NaCl. The anionic charge state of the adsorbed molecule [5] enables its direct excitation by a laser-induced gap plasmon. We show STM-PL photon maps of an individual molecule and small molecular clusters qualitatively comparable to STM-EL maps [5], but independent of the tunneling current. This brings a major advantage over electroluminescence as the current is a scaling factor in the photon map intensity and its elimination [5-7] creates unwanted artefacts.

[1] B. Yang et al. Nat. Photonics 14, 693 (2020). [2] H. Imada et al. Science 373, 95 (2021). [3] K. Kaiser et al. arXiv:2211.01051 (2022). [4] B. Doppagne et al. Science 361, 251 (2018). [5] J. Doležal et al. ACS Nano 16, 1082 (2022). [6] B. Doppagne et al. PRL 118, 127401 (2017). [7] Y. Zhang et al. Nature 531, 623 (2016).

O 76.6 Thu 11:45 WIL A317

A Setup for Fluorescence-Detected Two-Dimensional Electronic Spectroscopy of Single Molecules — •Sanchayeeta Jana, Simon Durst, Lucas Ludwig, and Markus Lippitz — Chair for Experimental Physics III, University of Bayreuth, Bayreuth, Germany

Fluorescence-Detected Two-Dimensional Electronic Spectroscopy is a recent ultrafast technique that yields information about the coupling between the states of a system. At the same time, fluorescence-detected single molecule spectroscopy is a well-established technique since more than 30 years. By combining these two techniques one should be able to measure 2d spectra of single molecules to get new insight in molecular dynamics on ultrashort time scales.

Here we present our work towards this goal. We use four phase-modulated ultrafast pulses to excite the molecule with the help of a high NA objective. The fluorescence is registered by single-photon detectors and demodulated at several mixing frequencies to get the rephasing and non-rephasing signals. The novelty of our technique is that we can measure Fluorescence Correlation Spectroscopy (FCS) and Time-Correlated Single Photon Counting (TCSPC) simultaneously to monitor the number of molecules in our excitation focus and the fluorescence lifetime.

In this work we illustrate our experimental technique and discuss 2d spectra measured on a molecular sample at low concentration.

O 76.7 Thu 12:00 WIL A317

Luminescence from Cu_2O films and bulk crystals in the STM — Alexander Gloystein, Mina Soltanmohammadi, and •Niklas Nilius — Carl von Ossietzky Universität, Institut für Physik, D-26111 Oldenburg, Germany

STM luminescence spectroscopy is employed to compare the optical response of bulk $Cu_2O(111)$ and 1-10 nm thick $Cu_2O/Au(111)$ films. Although both systems share similar structural and electronic properties and expose the same thermodynamically preferred $(\sqrt{3}\times\sqrt{3})R30^\circ$ reconstruction, their luminescence exhibits pronounced differences. The spectra of bulk Cu_2O are dominated by the recombination of free and defect-bound excitons, whereas a unique plasmonic response is detected for the oxide films. The latter arises from the electromagnetic coupling between STM tip and gold support, while the Cu_2O ad-layer exclusively controls the inelastic tunneling rates, i.e., the intensity, but not the spectral signature of the emission. Only upon tunneling into the Cu_2O band gap, a luminescence channel mediated by O vacancies is identified in the oxide film. The talk addresses the question why the unique exciton response of Cu_2O is covered by plasmon excitations even in films as thick as 10 nm.

O 76.8 Thu 12:15 WIL A317

Hot-carrier transfer across a nanoparticle-molecule junction: The importance of orbital hybridization and level alignment — •Jakub Fojt[1], Tuomas Rossi[2], Mikael Kuisma[3], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Department of Applied Physics, Aalto University, Aalto, Finland — [3]Department of Physics, Technical University of Denmark, Kongens Lyngby, Denmark

While direct hot-carrier transfer can increase photocatalytic activity, it is difficult to discern experimentally and competes with several other mechanisms. To shed light on these aspects, here, we model from first-principles hot-carrier generation across the interface between plasmonic nanoparticles and a CO molecule. The hot-electron transfer probability depends nonmonotonically on the nanoparticle-molecule distance and can be effective at long distances, even before a strong chemical bond can form; hot-hole transfer on the other hand is limited to shorter distances. These observations can be explained by the energetic alignment between molecular and nanoparticle states as well as the excitation frequency. The hybridization of the molecular orbitals is the key predictor for hot-carrier transfer in these systems, emphasizing the necessity of ground state hybridization for accurate predictions. Finally, we show a nontrivial dependence of the hot-carrier distribution on the excitation energy, which could be exploited when optimizing photocatalytic systems.

O 76.9 Thu 12:30 WIL A317

Disentangling the Orientations of Spectrally Overlapping Transition Dipoles in Dense Dye Layers — •Christoph Schnupfhagn[1], Thorsten Schumacher[1], Paul Markus[2], Georg Papastavrou[2], Olha Aftenieva[3], Tobias A. F. König[3], Volodymyr Dudko[4], Marian Matejdes[4], Josef Breu[4], and Markus Lippitz[1] — [1]Experimental Physics III, University of Bayreuth — [2]Physical Chemistry II, University of Bayreuth — [3]Leibniz-Institut für Polymerforschung Dresden e.V. — [4]Inorganic Chemistry I, University of Bayreuth

The transition dipole orientations of dye assemblies in heterostructures have a crucial impact on the efficiency of novel optoelectronic devices such as organic thin-film transistors and light-emitting diodes. These devices are frequently based on heterojunctions and tandem structures featuring multiple optical transitions. Precise knowledge of preferred orientations, spatial order, and spatial variations is highly relevant. We present a fast and universal large-area screening method to determine the transition dipole orientations in dye assemblies with diffraction-limited spatial resolution. Moreover, our hyperspectral imaging approach disentangles the orientations of different chromophores. As a demonstration, we apply our technique to dye monolayers with two optical transitions sandwiched between two ultrathin silicate nanosheets. A comprehensive model for dipole orientation distributions in monolayers reveals a long-range orientational order and a strong correlation between the two transitions.

O 77: Scanning Probe Techniques: Method Development II

Time: Thursday 10:30–12:45 Location: REC C 213

O 77.1 Thu 10:30 REC C 213

How cold is the junction of a millikelvin scanning tunnelling microscope? — Taner Esat[1,2], Xiaosheng Yang[1,2], Farhad Mustafayev[1,2], Helmut Soltner[3], Stefan Tautz[1,2,4], and •Ruslan Temirov[1,5] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Jülich, Germany — [3]Zentralinstitut für Engineering, Elektronik und Analytik (ZEA-1), Forschungszentrum Jülich, Germany — [4]Experimentalphysik IV A, RWTH Aachen University, Aachen, Germany — [5]University of Cologne, Institute of Physics II, Cologne, Germany

We employ a millikelvin scanning tunnelling microscope (STM) cooled to millikelvin temperatures by an adiabatic demagnetization refrigerator (ADR) to perform scanning tunnelling spectroscopy (STS) on an atomically clean surface of Al(100) in a superconducting state using normal-metal and superconducting STM tips. Varying the ADR temperatures between 30 mK and 1.2 K, we show that the temperature of the STM junction T is decoupled from the temperature of the surrounding environment T_{env}. Simulating the Josephson current with the $P(E)$ theory, we determine that $T_{\mathrm{env}} \approx 1.5$ K, while fitting of the superconducting gap yields the lowest $T \approx 77$ mK.

O 77.2 Thu 10:45 REC C 213

Ultrahigh Vacuum Scanning Tunneling Microscopy with z Resolution of 2 pm at 1.3 K using Combined Pulse Tube and Joule-Thomson Cooling — •Marcus Esser[1], Marc Frömming[1], Marco Pratzer[1], Michael Krzyzowski[2], and Markus Morgenstern[1] — [1]2.Physikalische Institut B, RWTH Aachen University, Aachen, Germany — [2]CryoVac GmbH & Co KG, Troisdorf, Germany

The cooling of scanning tunneling microscopes with liquid helium by bath or flux cryostats suffers from He losses that get increasingly expensive. However, alternative closed cycle systems based on pulse tube refrigerators can induce additional mechanical noise into the tunneling contact due to mechanical vibrations in the μm range and acoustic emissions. We will present an STM system that reaches temperatures of 1.3 K and a z resolution of 2 pm (feedback loop off) with the help of a pulse tube cooler and a Joule-Thomson stage. The challenge is to provide a good thermal coupling as well as an good vibration damping. For this purpose, a new concept with multiple decoupling stages including negative stiffness isolation, detached coaxially guided shields for the different temperature stages and an optimized conical microscope design made out of Shapal Hi M-soft has been realized. Numerical calculations of transfer functions are compared with measurements on test setups using accelerometers as well as the tunneling contact of the STM. Eventual measurements on Au(111) showed atomic resolution and mechanical vibrations below 2 pm. The ongoing work to optimize spectroscopic resolution will be reported.

O 77.3 Thu 11:00 REC C 213

Development of a closed-cycle dilution refrigerator scanning tunneling microscope — •Mate Stark[1], Daria Sostina[2], Wantong Huang[1], Paul Greule[1], Christoph Sürgers[1], Philip Willke[1], and Wolfgang Wernsdorfer[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology, Karlsruhe, Germany

Throughout the last decades, scanning probe techniques, such as scanning tunneling microscopy (STM), have been successfully paving the way to discover and understand physics on the atomic scale. However, recent developments in studying single atoms' electronic and magnetic properties have shown experimental limitations. For instance, the combination of electron spin resonance (ESR) with STM has shown short spin relaxation time T_1 and phase coherence time T_2 on single atoms, among others limited by thermally excited electrons [Willke et al., Sci. Adv. 4(2), 1543 (2018)].
Here, we present the implementation of a compact closed-cycle dilution refrigerator (DR) reaching milli-Kelvin temperatures, which we combine with a commercial STM under ultra-high vacuum (UHV) conditions. This combination enables a fast cool down, shows a low vibrational level, and requires a minimum of everyday maintenance. We demonstrate the functionality of the DR-STM by performing ESR measurements on individual magnetic molecules.

O 77.4 Thu 11:15 REC C 213

Machine learning: radical technique or plus ça change? The case for automated scanning probe microscopy — •Dylan Barker, Adam Sweetman, and Phil Blowey — University of Leeds

Atomic resolution scanning probe microscopy (SPM) provides a critical tool for studying the chemical and electronic structure of surfaces at the single atom scale, however, practically these techniques require a large amount of experimental time to manually prepare the scanning probe tip in-situ, usually via controlled indents into the surface. This apparently simple, but time-consuming process, is potentially an ideal candidate for automation using machine learning and computer vision techniques. Previous attempts to automate the classification of probe tips from topographical images have been made using machine learning methods [1-2], however using prior knowledge of the system in question we find it is also possible to classify the tip state using computationally simple image analysis methods such as Fourier ring correlation and cross-correlation. In this work I will present a comparison between "deterministic" image analysis methods and machine learning approaches for tip state classification. I will also address the known issue of small sample sizes for training ML techniques for SPM image classification, via an automated (scripted) data generation approach.

[1] Rashidi, M & Wolkow, R. A. ACS Nano 12, 5185-5189 (2018).

[2] Gordon, O. et al. Review of Scientific Instruments 90, 103704 (2019).

O 77.5 Thu 11:30 REC C 213

Artificial Intelligence finds the optimal STM manipulation parameters of unknown molecules — •Bernhard Ramsauer[1], Grant J. Simpson[2], Leonhard Grill[2], and Oliver T. Hofmann[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Department of Physical Chemistry, Institute of Chemistry, NAWI Graz, University Graz, Heinrichstraße 28, 8010 Graz, Austria

Scanning probe microscopy gives us the possibility to precisely control the position and orientation of single molecules and unlocks the possibility of nanofabrication of novel structures with enhanced properties. However, interaction processes at the nanoscale are stochastic processes, and because their motion itself is often unintuitive and hard to predict, inducing controlled movements is not trivial at all.

In this study we present how a reinforcement learning algorithm identifies optimal manipulation parameters (i.e., the bias voltage, height, and lateral position of the STM tip relative to the molecule) for any unknown molecule to allow for precise control of its movement.

Leaving all the manipulation parameters open for investigation requires a method to exclude manipulation parameter that pick-up or destroy the molecule. Furthermore, already learned information is used to infer prior knowledge to similar manipulation parameters (e.g.: to infer knowledge at the same bias voltage to adjacent tip positions).

This allows for autonomous control of initially unknown molecules with high sub-nanometer precision that set the basis to construct molecular nanostructures from the bottom up.

O 77.6 Thu 11:45 REC C 213

Field-emission resonances at exceptional large voltages: Consequences for determining work functions — •Anika Schlenhoff[1], Gerassimos C. Kokkorakis[2], and John P. Xanthakis[2] — [1]Institute of Physics, University of Münster, Germany — [2]Electrical and Computer Engineering Department, National Technical University of Athens, Greece

In a scanning tunneling microscopy (STM) setup, a series of unoccupied electronic states evolve in the vacuum gap between the probe tip and the surface. Due to limited bias voltage ranges, so far only a small number (typically 4 - 8) of these so-called field-emission resonances (FERs) have been detected. Here, we report a combined experimental and theoretical study of FERs over an exceptional range of energy and number, typically tens of an eV and over thirty in order n [1]. Unlike commonly assumed, the triangular potential well is not found to be a good approximation for the high-n states. Although the spectroscopy mode assures a constant electric field at the tip apex, this leads only for the intermediate FERs (approx. $2 < n < 6$) to reside in a linear potential between the tip and the surface. At higher tip-sample distances d and bias voltages $U(d)$, the quantum well is no longer triangular but attains a curvature, which is d-dependent. Each high-n state resides in its own well that can be well-approximated by a polynomial of second order. Hence, the range of U_n to be analyzed in terms of spectroscopic positions needs to be chosen with great care when deducing surface work functions.
[1] A. Schlenhoff *et al.*, Appl. Phys. Lett. **120**, 261601 (2022).

O 77.7 Thu 12:00 REC C 213

Phase compensation for ultrafast dynamic measurements of atomic spins — •Nicolaj Betz[1], Max Hänze[1,2], Gregory McMurtrie[1], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Understanding spin dynamics is vital for a wide range of applications , such as qubit manipulation. However, in many cases, especially for single atoms on surfaces, even stroboscopic measurement techniques, like pump-probe or pulsed electron spin resonance, do not provide enough time resolution to resolve the dynamics of the individual (atomic) spins. Such measurements are generally limited by the attenuation and distortion of the sharp pulses, that inevitably occurs due to imperfections in the instrumental setup. The attenuation in the frequency domain can be measured and compensated for [M. Herve, et al. Appl. Phys. Lett. 107, 093101, 2015]. However, such a compensation only has limited impact on the distortion. Here, we introduce a new technique, that enables the measurement of the phase shift between individual frequencies directly in the tunnel junction of a scanning tunneling microscope (STM). Using these phase shifts it is now possible to fully compensate arbitrary pulses and manipulate atomic spins with picosecond time resolution. Phase information also provides additional insights into stochastic resonance, an effect we recently utilized as an alternative way to measure spin dynamics [M. Hänze, et al. Sci. Adv. 7, 33, 2021], even of multiple spin states.

O 77.8 Thu 12:15 REC C 213

Simultaneous Measurement of Quasiparticle Interference and Decay Length Using Parallel Spectroscopy with the Scanning Tunneling Microscope — •Berk Zengin, Danyang Liu, Aleš Cahlík, Kevin Hauser, and Fabian D. Natterer — University of Zurich, Department of Physics, Winterthurerstrasse 190, 8057 Zurich, Switzerland

Developments in signal processing unlock the possibility to perform significantly faster spectroscopic measurements with a Scanning Tunneling Microscope by utilizing the harmonics created by non-linearities in the current-voltage characteristics. Having the capability to perform spectroscopy on the order of few milliseconds to measure the local density states(LDOS), we can afford to additionally vary the tip sample distance during QPI mapping, providing spatially and energy resolved decay length information. Our work shows how LDOS and decay length mapping can yield valuable insight into the electronic structure and dispersion relation of surface electrons.

O 77.9 Thu 12:30 REC C 213

Unveiling interference of Yu-Shiba-Rusinov states with novel multi-functionalized STM probe — •Artem Odobesko, Felix Friedrich, and Mathias Bode — Physikalisches Institut, Universität Würzburg, 97074, Würzburg, Germany

Scattering of superconducting pairs by magnetic impurities on superconducting surface results into pairs of sharp ingap resonances, known as Yu-Shiba-Rusinov states. By analogue with interference of quasiparticles scattered by defects in normal metals, these excitations form periodic charge density texture around magnetic impurity. Typically, STM is equipped with a superconducting (SC) probe to increase the energy resolution bypassing thermal broadening to detect these states. However, with such STM probe it almost unattainable to observe the spatial oscillatory behavior of YSR wave function due to a very fast spatial attenuation away from the impurity (with decay ~ 1/r). In this work, we attach a CO molecule to a SC-probe to maximize simultaneously both spatial and energy resolution. We examine the LDOS distribution of YSR states around the magnetic Fe dimer on Nb(110). The last leads to hybridization of YSR states, which can be interpreted as symmetric and antisymmetric combinations of YSR excitation of an individual Fe impurity. Using such CO-SC-probe we are able to map both symmetric and antisymmetric oscillatory interference patterns of hybridized YSR states in vicinity of Fe dimer. Compared to measurements made with CO-free probe, we demonstrate an exceptional spatial sensitivity combined with high energy resolution with a new multi-functionalized probe.

O 78: Heterogeneous Catalysis and Surface Dynamics II

Time: Thursday 10:30–12:45 Location: TRE Phy

O 78.1 Thu 10:30 TRE Phy

Data-centric heterogeneous catalysis: identifying rules and materials genes of alkane selective oxidation — •Lucas Foppa[1], Frederik Rüther[2], Michael Geske[2], Gregor Koch[3], Frank Girgsdies[3], Pierre Kube[3], Spencer J. Carey[3], Michael Hävecker[4], Olaf Timpe[3], Andrey Tarasov[3], Matthias Scheffler[1], Frank Rosowski[2], Robert Schlögl[3,4], and Annette Trunschke[3] — [1]The NOMAD Lab. at the FHI of the MPG and IRIS-Adlershof of HU Berlin — [2]BasCat Lab. at TU Berlin — [3]FHI of the MPG — [4]Max Planck Institute for Chemical Energy Conversion

Artificial Intelligence (AI) can accelerate materials design by identifying the key parameters correlated with the performance. However, widely used AI methods require big data, and only the smallest part of catalysis-research data meets the quality requirement for data-efficient AI. We use rigorous experimental procedures[1] to measure 55 physicochemical parameters as well as the reactivity of 12 catalysts towards ethane, propane, and n-butane oxidation. By applying the sure-independence-screening-and-sparsifying-operator approach to the so-obtained data set, we identify nonlinear property-function relationships depending on several key parameters and reflecting the intricate interplay of processes governing selective oxidation.[2,3]

[1] A. Trunschke, *et al.*, *Top. Catal.* **63**, 1683-1699 (2020).
[2] L. Foppa, *et al.*, *MRS Bull.* **46**, 1 (2021).
[3] L. Foppa, *et al.*, *ChemRxiv*, 10.26434/chemrxiv-2022-xmg75 (2022).

O 78.2 Thu 10:45 TRE Phy

Adaptive Experimental Designs for the Unsupervised Exploration of Reaction Kinetic Phase Diagrams — •Frederic Felsen, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin, Germany

In heterogeneous catalysis the interplay of various elementary processes taking place at the catalytic interface gives rise to complex kinetic phase diagrams [1]. Characteristic for such phase diagrams are regimes of smooth kinetic behavior separated by phase transitions going along with drastic changes in effective kinetics. Generally it is difficult to reconstruct the kinetic regime topology of a given process without a detailed understanding of the underlying reaction mechanism. Here, we tackle this issue by approximating the reaction kinetics using statistically robust effective rate laws [2]. Locally fingerprinting the apparent behavior of a chemical reaction, we can generate point-wise regime labels as a basis for estimates of the position of the phase transitions. In order to achieve this in a data efficient way, we propose an iterative adaptive design algorithm, bridging between the classical theory of experimental design [3] and modern statistical learning and optimization. Using a microkinetic model, we illustrate the potential of this approach by investigating the kinetic phase diagram of CO oxidation over RuO_2.

[1] V. Zhdanov et al., Surf. Sci. Rep. **20**, 113, (1994).
[2] F. Felsen et al., Chem. Eng. J. **433**, 134121, (2022).
[3] V. Fedorov, *Theory of Optimal Experiments* (1972).

O 78.3 Thu 11:00 TRE Phy

Machine-learning Gaussian Approximation Potentials to discover RuO_2 surface reconstructions — •Yonghyuk Lee, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

Machine-learning Gaussian Approximation Potentials (GAPs) have recently evolved into a powerful class of surrogate models for computationally demanding first-principles calculations. Combined with structure exploration techniques, they enable us to examine the potential energy surface of interest with a hitherto unforeseen combination of physical accuracy and computational efficiency and to achieve global surface structure determination (SSD) for increasingly complex systems. This can be exploited, e.g., to discover novel surface motifs, which are critical in understanding the dynamics of heterogeneous catalysts under operating conditions. In our preceding study on IrO_2, this methodology was extended by a general and data-efficient active-learning framework that allows for the on-the-fly generation of GAPs via the actual surface exploration process. During the iterative GAP refinement for RuO_2, we have now identified plenty of unknown low-energy reconstructions of RuO_2 low index facets. Intriguingly, by extending the searching space to larger surface unit cells, we discovered $c(2\times2)$ reconstructions of $RuO_2(100)$, which provide solutions to long-standing questions in heterogeneous catalysis and experiments.

[1] J. Timmermann *et al.*, Phys. Rev. Lett. **125**, 206101 (2020)
[2] J. Timmermann *et al.*, J. Chem. Phys., **155**, 244107 (2021)

O 78.4 Thu 11:15 TRE Phy

Exploration of IrO2 electrocatalyst deactivation via machine learning potentials — •Hao Wan, Hendrik Heenen, Simon Wengert, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

IrO2 catalysts are one of the best performing oxygen evolution reaction (OER) catalysts in terms of both catalytic activity and stability under harsh acidic conditions. Yet, they still suffer from deactivation under long term OER conditions due to possible changes in surface compositions and morphology. To shed light into these deactivation processes, characterization of the microscopic structure and composition of IrO2 interfaces is necessary. The involved phase space, however, is vast and its exploration requires extensive sampling and automatic (surface) structure searches which are unfeasible via Density Functional Theory (DFT) calculations. Enabling the intensive computations, machine learning interatomic potentials (MLIP) retain DFT accuracy to within a few meV per atom while reducing the computational cost by up to three orders of magnitude.

In this contribution, we present a reliable MLIP based on Gaussian approximation potentials to investigate IrO2 deactivation. Stable and metastable IrO2 surfaces at various surface oxidation states have been extensively sampled using parallel tempering. Relevant surfaces are suggested by evaluating their relative stability compared to rutile-IrO2(110), while considering electrochemical conditions. OER activity from these surfaces can be estimated using established reaction descriptors which will help unravel likely deactivation mechanisms.

O 78.5 Thu 11:30 TRE Phy

Machine Learning Driven Molecular Dynamics Simulation of the M1 Selective Oxidation Catalysts — •Kyeonghyeon Nam[1], Yonghyuk Lee[1], Liudmyla Masliuk[2], Thomas Lunkenbein[2], Annette Trunschke[2], Christoph Scheurer[1], and Karsten Reuter[1] — [1]Theory, Fritz-Haber-Institut der MPG — [2]Inorganic Chem. Dept., Fritz-Haber-Institut der MPG, Berlin, Germany

The activity and selectivity of realistic heterogeneous catalysts can be altered noticeably by small changes in a multitude of factors such as bulk composition, dopants, defects, reaction conditions, etc. Their effects are furthermore interrelated in non-trivial ways. As an important first step to rationally disentangle them, we here aim to understand their influences on the evolution of local atomic-scale structural motifs presented by the catalyst. Specifically, we do this for the M1 structural modification of $(Mo,V)O_x$ and $(Mo,V,Te,Nb)O_x$ as an active catalyst for oxidative dehydrogenation of ethane to ethylene. The large primitive cell of the M1 catalyst challenges a detailed study of all surface terminations by means of predictive-quality first-principles calculations. To this end, we deconstruct the primitive cell into 'rod-like structures' of surface motifs with various oxygen content. A machine-learned Gaussian Approximation Potential (GAP), trained against this structural library, faithfully reproduces experimental data from electron microscopy [1]. MD simulations of M1 catalyst hk0 prismatic faces with the iteratively improved GAP help to rationalize the influence of vanadium and niobium doping on the active surface structure.

[1] L. Masliuk *et al.*, J. Phys. Chem. C **121**, 24093 (2017).

O 78.6 Thu 11:45 TRE Phy

Studing of rate-limiting steps on CO_2 reduction on ZnO/Cu(111)

— •Sina Dortaj[1,2] and Sebastian Matera[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Institute for Mathematics, Freie Universität, Berlin, Germany

To simulate the chemical kinetics of heterogeneous catalysts, the kinetic Monte Carlo (kMC) method is a common choice as it allows estimating turnover frequencies and coverages with a tunable accuracy. This advantage comes at much higher computational costs compared to classical kinetic approaches, in addition to stochastic noise on the simulation results. Thus, local sensitivity analysis to determine the rate-limiting step becomes cumbersome. Additionally, rate constants often carry some sizeable uncertainty due to the intrinsic approximations in quantum chemical methods or the noise in experimental data used to determine reaction barriers that make the use of just local methods obscure. We address both problems, high costs, and parameter uncertainties, by a novel global sensitivity analysis based on the Cramér von Mises distance and a Quasi-Monte Carlo sampling of the space of rate constants. While applicable to any model, our approach is particularly suited for the use of kMC and other Monte Carlo models. We demonstrate the approach on the CO_2 reduction on ZnO/Cu(111) catalysts identifying the key atomic scale factors controlling activity and selectivity.

O 78.7 Thu 12:00 TRE Phy

Identifying materials genes describing selectivity of catalytic CO_2 hydrogenation: an AI approach with theoretical and experimental data

— •Ray Miyazaki[1], Kendra Belthle[2], Harun Tüysüz[2], Lucas Foppa[1], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin, Germany — [2]Max-Planck-Institut für Kohlenforschung, Germany

Investigating CO_2 hydrogenation by heterogeneous catalysis that mimics hydrothermal vents leads to a deeper understanding of the origin of organic molecules at the early earth [1]. We focus on cobalt nanoparticles supported on M-SiO_2 where hetero atoms (e.g., Ti or Al) are incorporated into SiO_2. However, heterogeneous catalysis is governed by an intricate interplay among multi-scale processes. Thus, it is rather difficult, if not impossible, to identify the key physical parameters correlated with the catalytic performance (*materials genes*) directly by theoretical or experimental approaches. In this study, materials properties obtained from density functional theory calculations and experiments, such as adsorption energy of CO_2 and measured pore volume, are used to model the experimental selectivity of each organic molecule (e.g., CH_3OH, CH_4) by the sure-independence screening and sparsifying operator (SISSO) AI approach [2]. In order to accelerate catalyst design, we also investigate the accuracy of the models using input parameter sets with the different acquisition cost.

[1] K. S. Belthle *et al.*, *J. Am. Chem. Soc.*, in press (2022).

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

O 78.8 Thu 12:15 TRE Phy

Structural and Electronic Properties of Iron Nanoparticles onto Well-Defined Ceria Thin Films

— •Lesia Piliai[1], Mykhailo Vorokhta[1], Peter Matvija[1], Tomáš Skála[1,2], Ivan Khalakhan[1], and Iva Matolínová[1] — [1]Charles University, Prague, Czech Republic — [2]Elettra-Sincrotrone, Elettra-Sincrotrone, Italy

The interaction of iron with ceria using model Fe/ceria systems consisting of Fe nanoparticles vapor deposited on well-ordered CeOx(x=1,5;2) thin films grown on Cu(111) has been investigated by X-ray photoelectron spectroscopy (XPS), synchrotron radiation photoemission spectroscopy (SRPES), and scanning tunneling microscopy (STM). The Fe atoms are oxidized to Fe3+ and Fe2+ species upon deposition on CeO2 at 300 K at the cost of the reduction of Ce4+ to Ce3+. With increasing the Fe coverage, the concentration of Ce3+ increases monotonically. The notable growth of Fe2+ species was observed upon deposition on CeO2 at 300 K, but Fe3+ species remain predominant in Fe/CeOx systems. Our studies demonstrate that in comparison with other transition metals, Fe remains oxidized on ceria even at higher coverage and exhibits a small particle size, likely arising from strong metal*support interactions. Combining the SRPES and STM data suggests that annealing to higher temperatures leads to the formation of an iron-ceria solid solution. These results illustrate that Fe modifies both the electronic and structural properties of ceria depending on external conditions.

O 78.9 Thu 12:30 TRE Phy

In situ characterization of cerium oxide on Au(111) under reducing and oxidizing conditions by low-energy electron microscopy

— •Rudi Tschammer[1], Lars Buss[1,2], Carlos Morales[1], Sanjaya Senanayake[3], Jens Falta[2,4], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Institute of Solid State Physics, University of Bremen, Bremen, Germany — [3]Chemistry Division, Brookhaven National Laboratory, Upton, NY 11973, USA — [4]MAPEX Center for Materials and Processes, University of Bremen, Bremen, Germany

The development of novel catalysts for a variety of applications is a key challenge for modern catalysis. Inverse metal oxide catalysts consisting of oxide nanoparticles dispersed on a metal support have recently attracted much attention, showing higher activity and selectivity compared to traditional catalytic systems, harnessing synergistic effects attributed to the so-called metal-support interaction. To gain further insights, we deposited cerium oxide nanoparticles on Au(111) and studied this system by low-energy electron microscopy (LEEM) and low-energy electron diffraction (LEED). The prepared samples demonstrate a distinct correlation between the deposition temperature and the structural order of the nanoparticles. This has been expanded upon by exploring the changes induced by reduction with H_2 and reoxidation with O_2 or CO_2, again exhibiting a connection between structural order and activity, while also showing the influence of the oxide-metal interaction on the stability of cerium oxide under reducing conditions.

O 79: Focus Session: Frontiers of Electronic-Structure Theory VI (joint session O/HL)

Time: Thursday 10:30–12:45 Location: TRE Ma

O 79.1 Thu 10:30 TRE Ma

Nailing down charge-density-wave phase-transition temperatures with downfolding approaches — •Arne Schobert[1], Jan Berges[2], Michael Sentef[3], Erik van Loon[4], Sergey Brener[1], Mariana Rossi[3], and Tim Wehling[1] — [1]University of Hamburg, Germany — [2]University of Bremen, Germany — [3]MPSD, Hamburg, Germany — [4]Lund University, Sweden

The coupled dynamics of electrons and nuclei is an extremely complex problem of relevance to multiple branches of sciences. *Ab initio* molecular dynamics (AIMD) simulations are often challenging — especially in large systems, on long time scales, in non-equilibrium or in presence of strong correlation. We can overcome these problems by mapping the full *ab initio* density functional theory (DFT) Hamiltonian onto a low-energy lattice model through downfolding. Three different downfolding strategies based on constraining, unscreening and combinations thereof are compared. The best performing model, which properly accounts for anharmonicity, is combined with path integral molecular dynamics (PIMD). This allows us to nail down the transition temperatures of charge-density waves — for instance in 1H-TaS$_2$.

O 79.2 Thu 10:45 TRE Ma

Structural and electronic properties of the Ba$_8$Au$_x$Ge$_{46-x}$ clathrate: an ab-initio study with cluster expansion — •Peter Weber, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Germany

Intermetallic clathrate materials are promising candidates for high-efficiency thermoelectric applications as they can reach very low thermal conductivity. These materials possess a cage-like structure containing guest atoms. Their electronic properties can be tailored by exploiting the idea of the phonon-glass–electron-crystal which allows for reaching a large figure of merit. We study the compound Ba$_8$Au$_x$Ge$_{46-x}$ ($0 \leq x \leq 8$), which has raised interest due to its glass-like thermal conductivity [1]. Using the Zintl concept, a semiconducting state is expected to occur at the charge-balanced composition corresponding to x=5.33. This composition requires a supercell of at least 3 unit cells (162 atoms) which makes a direct *ab initio* study challenging. We tackle this problem by using the cluster expansion method combined with density-functional theory calculations. In this way, we are able to find the atomic ground-state configurations, together with various properties at different temperatures and gold content. These include lattice constants, bond lengths, site occupancies, as well as band gaps and band structures which are compared with available experimental data.

[1] P.-F. Lory, *et al.* Nature Communications **8**, 491 (2017).

Topical Talk O 79.3 Thu 11:00 TRE Ma

New Opportunities for First Principles Simulations of Thousands of Atoms Using Linear Scaling Density Functional Theory — •Laura Ratcliff — University of Bristol, Bristol, United Kingdom

Density-functional theory (DFT) is routinely used to simulate a wide variety of materials and properties, however, standard implementations are cubic scaling with the number of atoms, limiting the system sizes which can be treated. This motivated the development of alternative implementations of DFT, which exploit the nearsightedness principle by using a localised description of the system, leading to algorithms with linear scaling (LS) cost which can treat large systems containing tens of thousands of atoms. One approach, which is implemented in the wavelet-based BigDFT code, uses localised orbitals, also known as support functions, which are optimised to reflect their local chemical environment, and thus constitute an accurate minimal basis set. Beyond reduced computational cost, the localised support function description also facilitates additional developments, such as the ability to automate a fragment-based description. In this talk we will present the formalism behind LS-BigDFT, including some examples of the new types of systems and analyses which are opened up by the ability to treat such large systems. We will also describe recent developments in PyBigDFT, a python-based interface which aims to simplify the usage of LS-BigDFT for complex systems and workflows.

15 min. break

O 79.4 Thu 11:45 TRE Ma

Fully Anharmonic Electronic Transport Coefficients from Temperature-dependent Spectral Functions — •Jingkai Quan, Matthias Scheffler, and Christian Carbogno — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin

The combination of *ab initio* molecular dynamics (aiMD) and band-structure unfolding techniques provides a non-perturbative route to obtain temperature-dependent spectral functions. [1] In contrast to commonly employed perturbative approaches [2], this technique accounts for all orders of anharmonic and vibronic couplings. Building on this non-perturbative formalisms, we here present an approach to obtain electronic transport coefficient such as the electrical conductivity using Kubo's formulation of the fluctuation-dissipation theorem. By this means, all relevant quantities, including electron lifetimes, are obtained from the unfolded, self-consistent wave functions computed during the aiMD runs. We critically benchmark the approach against existing perturbative data for harmonic systems, carefully analyzing to which extent short- and long-range couplings are captured with increasing supercell size. Furthermore, we demonstrate the advantages of the proposed approach for strongly anharmonic systems, for which perturbative approaches become unreliable.

[1] M. Zacharias, M. Scheffler, and C. Carbogno, *Phys. Rev. B* **102**, 045126 (2020).

[2] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).

O 79.5 Thu 12:00 TRE Ma

Accurate prediction of vibrational spectra for solid state systems from ab initio molecular dynamics — •Ekin Esme Bas, Thomas Heine, and Dorothea Golze — Chair of Theoretical Chemistry, Technische Universität Dresden, 01062 Dresden, Germany

We present a highly accurate computational method to calculate vibrational spectra for solid state materials, primarily for covalent-organic frameworks (COFs). IR and Raman spectra are important tools that are frequently used for material characterization. However, the experimental spectra are often difficult to interpret without aid from theory. The computation of IR and Raman spectra is usually based on the harmonic approximation where molecular vibrations can be determined as normal modes from the second derivatives of the electronic energy with respect to the coordinates. Although this method is more straightforward and computationally less expensive, anharmonic modes cannot be captured. Thus, we employ an AIMD (ab initio molecular dynamics) based approach to include vibrational anharmonicities. Power, IR and Raman spectra can then be calculated via a Fourier transformation of the time correlation functions of velocities, dipole moments and polarizability tensors, respectively [1]. We discuss different approaches to compute dipole moments and polarizabilities. We present the power, IR and Raman spectra we calculated for COF-1, and we compare our AIMD based approach to the spectra obtained via harmonic approximation and experiment.

[1] M. Thomas, M. Brehm, R. Fligg, P. Vöhringer, B. Kirchner. Phys. Chem. Chem. Phys., 6608-6622, 5, 2013.

O 79.6 Thu 12:15 TRE Ma

Anharmonic Fingerprints from THz Modes of Polyacene Crystals — •Paolo Lazzaroni, Shubham Sharma, and Mariana Rossi — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Organic molecular crystals exhibit strong lattice anharmonicity, especially in the collective motions that are governed by intermolecular interactions and lie in the low-frequency THz range [1]. Inspired by recent observations that the polarization-orientation (PO) Raman spectra can give exquisite insight into the anharmonic couplings between modes [2], we devise a first-principles framework that can reproduce, explain and give quantitative insight into the type and strengths of mode coupling. This framework is based on machine-learned potentials and polarizability tensors trained on *ab initio* molecular dynamics trajectories [3]. We obtain results through the time-correlation formalism for PO Raman signals, retaining the full anharmonic nature of the potential, and perform a novel analysis of effective temperature-dependent mode couplings from our trajectories. [1] M. Asher *et al.*, Adv. Mater. **32**, 1908028 (2020) [2] N. Benshalom *et* *al.*, arXiv:2204.12528 (2022) [3] N. Raimbault *et al.*, *New J. Phys.* **21** 105001 (2019)

O 79.7 Thu 12:30 TRE Ma

A first-principles Newns-Anderson chemisorption function applied to ultrafast electron transfer — •Simiam Ghan[1], Elias Diesen[1], Christian Kunkel[1], Karsten Reuter[1], and Harald Oberhofer[2] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany. — [2]University of Bayreuth, Bayreuth, Germany

We offer a method to calculate the electronic couplings H_{ad} between an adsorbate and substrate in an ab-initio fashion. The couplings are acquired by projection of the Kohn-Sham Hamiltonian onto a diabatic basis[1]. By averaging over the Brillouin Zone, it becomes possible to calculate a convergent chemisorption function of Newns and Anderson[2], which gives the energetic broadening of an adsorbate frontier orbital upon adsorption. This broadening corresponds to the experimentally-observable lifetime of an electron in the state, which we confirm for the case of core-excited $\mathrm{Ar}^*(2p^{-1}_{3/2}4s)$ atoms on a number of transition metal surfaces[3].

We find that the (tunneling) model captures and elucidates aspects of energy-dependence, spin, phase cancellation and k-space in the electron transfer process, in particular suggesting a significant role played by the surface d-bands. Given the prevalence of electronic couplings - and the chemisorption function - in theoretical models, we discuss potential for further applications.

[1] S. Ghan et al., J. Chem. Theory Comput. **16**, 7431 (2020).

[2] D. Newns, Phys. Rev. **178**, 3, 1123 (1969).

[3] F. Blobner et al., Phys. Rev. Lett. **112**, 086801 (2014).

O 80: Plasmonics and Nanooptics IV: Light-Matter Interaction and Spectroscopy III

Time: Thursday 15:00–17:15 Location: CHE 89

O 80.1 Thu 15:00 CHE 89

Energy and momentum distribution of surface plasmon-induced hot carriers — •Christopher Weiss[1], Michael Hartelt[1], Pavel N. Terekhin[1], Tobias Eul[1], Anna-Katharina Mahro[1], Benjamin Frisch[1], Eva Prinz[1], Baerbel Rethfeld[1], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, Germany

Are the spectroscopic properties of plasmon- and photon-induced hot carriers fundamentally different? Electrons excited at the bulk plasmon resonance, for example, exhibit a distinct spectroscopic signature [1]. However, bulk plasmons are rather unsuited for technological applications compared to surface plasmons.

To answer the initial question for surface plasmons, we separate the energy and momentum distributions of surface plasmon polariton (SPP)-induced hot electrons from those of photoexcited electrons in a two-color time-resolved photoemission electron microscopy experiment.

In our experiment, these SPP-induced hot electrons show only small momenta parallel to the surface and a narrow energy distribution close to the Fermi energy [2]. This result clearly distinguishes them spectroscopically from their photoinduced counterparts.

[1] Reutzel et al., Phys. Rev. Lett. 123 (2019), 017404

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

O 80.2 Thu 15:15 CHE 89

Lorentz Microscopy of Optical Fields — •John H. Gaida[1,2], Hugo Lourenço-Martins[1,2], Sergey V. Yalunin[1,2], Armin Feist[1,2], Murat Sivis[1,2], Thorsten Hohage[3], F. Javier García de Abajo[4,5], and Claus Ropers[1,2] — [1]MPI for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany — [3]Institute of Numerical and Applied Mathematics, University of Göttingen, Germany — [4]ICFO-Institut de Ciencies Fotoniques, Castelldefels (Barcelona), Spain — [5]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain

In electron microscopy, detailed insights into nanoscale optical properties of materials are gained by spontaneous inelastic scattering leading to electron-energy loss and cathodoluminescence. Photon-induced near-field electron microscopy (PINEM) allows for mode- and polarization-selective imaging based on stimulated scattering in the presence of external sample excitation. Through this process a spatial phase profile inherited from the optical fields is imprinted onto the wave function of the probing electrons. Here, we introduce Lorentz-PINEM for the full-field, non-invasive imaging of complex optical near fields at high spatial resolution. We use energy-filtered defocus phase-contrast imaging and iterative phase retrieval to reconstruct the phase distribution of interfering surface-bound modes on a plasmonic nanotip. Our approach is universally applicable to retrieve the spatial phase of nanoscale fields and topological modes.

[1] John H. Gaida, *et al.*, 2022, Preprint at Research Square *doi.org/10.21203/rs.3.rs-2150760/v1.*

Topical Talk O 80.3 Thu 15:30 CHE 89

Topological Plasmonics and Plasmonic Twistronics: Skyrmions, Merons, Quasicrystals, and Sykrmion Bags — •Harald Giessen[1], Bettina Frank[1], Pascal Dreher[2], David Janoschka[2], Frank Meyer zu Heringdorf[2], Julian Schwab[1], Tim Davis[1,4], Kobi Cohen[3], Shai Tsesses[3], and Guy Bartal[3] — [1]4. Physikalisches Institut, Universität Stuttgart, Germany — [2]CENIDE, University of Duisburg-Essen, Germany — [3]Technion, Haifa, Israel — [4]University of Melbourne, Australia

We present ultrafast vectorial electric field measurements of plasmonic skyrmions, merons, quasicrystalline structures, and skyrmion bags. 10 nm spatial resolution, sub-fs temporal resolution, and vectorial properties of the surface plasmon field on single crystalline, atomically flat gold surfaces are presented. Our techniques combine ultrafast vector PEEM and interferometric s-SNOM. Our tailored model systems reveal a rich set of topological phenomena, reaching even into 4-dimensional topology.

O 80.4 Thu 16:00 CHE 89

Direct imaging of photonic band-edge states in golden-angle Vogel spirals using photoemission electron microscopy — Martin Aeschlimann[1], Felix Fenner[2], Tobias Brixner[3], Benjamin Frisch[1], Patrick Folge[4], Michael Hartelt[1], •Matthias Hensen[3], Thomas H. Loeber[5], Walter Pfeiffer[2], Sebastian Pres[3], and Bernd Stannowski[6] — [1]Fachbereich Physik and Research Center OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany — [3]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, 97074 Würzburg, Germany — [4]Angewandte Physik, Universität Paderborn, 33098 Paderborn, Germany — [5]Nano-Structuring-Center, 67663 Kaiserslautern, Germany — [6]5PVcomB, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

Golden-angle Vogel spirals, as deterministic aperiodic structures, support isotropic photonic band gaps and have interesting applications. Especially localized modes, such as band-edge states, are essential for tailored light–matter interaction. Here we report imaging of such modes using photoemission electron microscopy (PEEM). Tunable ultrashort light pulses excite them in golden-angle Vogel spirals that were fabricated by focused-ion-beam (FIB) milling of an a-Si:H layer. The local near-field leads to electron emission which is detected spatially resolved. The demonstration of FIB-textured a-Si:H as photonic material and the ability of PEEM mode imaging offers means to spatiotemporally resolve mode dynamics and to perform nanospectroscopy.

O 80.5 Thu 16:15 CHE 89

Short-range plasmonic skyrmions — •Bettina Frank[1], Simon Mangold[1], Harald Giessen[1], Pascal Dreher[2], Frank Meyer zu Heringdorf[2], and Stefan Kaiser[1] — [1]4. Physikalisches Institut, Universität Stuttgart, Germany — [2]CENIDE, University of Duisburg-Essen

We utilize ultrathin, atomically flat, single crystalline gold flakes which compress the plasmon wavelength to lambda_air/7. Using hexagonal boundaries that are carved with focused gold ions, we demonstrate plasmonic skyrmions, both using PEEM as well as s-SNOM. The electromagnetic field is structured on a 140 nm scale, which offers opportunities for topological light-matter interaction on a deep subwavelength scale.

O 80.6 Thu 16:30 CHE 89

Phase-resolved mapping of plasmonic resonances at nanostructures — •Tim Dauwe[1,2], Hugo Lourenco-Martins[1,2], Murat Sivis[1,2], Jakob Hagen[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany — [2]IV. Physical Institute, University of Göttingen, 37077 Göttingen, Germany

In this contribution, we study resonant plasmonic nanostructures by a combination of inelastic electron-light scattering techniques. We investigate metallic nanorods using electron-energy loss spectroscopy (EELS) and photon-induced near-field electron microscopy (PINEM), elucidating spectrally-dependent mode profiles and symmetries using spontaneous and stimulated interactions. We explore multicolor excitation and nonlinear wave mixing as contrast mechanisms accessing spatial phase profiles and local nonlinear response.

O 80.7 Thu 16:45 CHE 89

Shortcut to Self-Consistent Light-Matter Interaction and Realistic Spectra from First Principles — •Christian Schäfer[1,2] and Göran Johansson[1] — [1]Department of Microtechnology and Nanoscience, MC2, Chalmers University of Technology, 412 96 Göteborg, Sweden — [2]Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

Nanoplasmonic and optical cavity environments provide a novel handle to non-intrusively control materials and chemistry. We introduce here a simple approach to how an electromagnetic environment can be efficiently embedded into state-of-the-art electronic structure methods, taking the form of radiation-reaction forces [1]. We demonstrate that this self-consistently provides access to various optical effects and provides an efficient path to connect vastly different system scales [2]. As an example, we illustrate its seamless integration into time-dependent density-functional theory and its application to polaritonic chemistry with virtually no additional cost, presenting a convenient shortcut to self-consistent light-matter interactions.

[1] C. Schäfer and G. Johansson, PRL 128, 156402 (2022).

[2] C. Schäfer, J. Phys. Chem. Lett. 2022, 13, 6905-6911.

O 80.8 Thu 17:00 CHE 89

Microscopic description of the optical response in metal nanoparticles — •Jonas Grumm, Robert Salzwedel, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany

The optical response of metal nanoparticles is dominated by the formation of collective electronic resonances, so-called localized plasmons.

Here, we present a microscopic approach to their temporal dynamics based on the self-consistent treatment of the microscopic Boltzmann transport equations and the macroscopic Maxwell's equations for the electromagnetic fields. The corresponding numerical simulations describe the formation, propagation and thermalization dynamics of plasmons via the coupled electron-phonon dynamics in the self-consisting solved optical field. The formalism allows nonlinear optical processes to be included in the description.

O 81: Oxide and Insulator Surfaces I: Adsorption and Reaction of Small Molecules

Time: Thursday 15:00–18:00 Location: CHE 91

O 81.1 Thu 15:00 CHE 91

Adsorption of phosphonic acids on Fe_3O_4 (001) surfaces - a DFT study — Wernfried Mayr-Schmölzer, Johann Fleischhaker, Somak Banerjee, Kai Sellschopp, and •Gregor Vonbun-Feldbauer — Institute of Advanced Ceramics, TU Hamburg, Germany

The usage of magnetite nanoparticles is interesting for diverse applications from catalysis to hybrid materials. In organic-inorganic hybrids, organic linker molecules are used to allow for the self-assembly of functionalized nanoparticles. The impact of linkers with different functional groups on the, e.g., mechanical properties of assembled materials is not fully clear yet. Here, we present results from investigating the adsorption of small phosphonic acids on the magnetite (001) surface using density functional theory calculations to shed light on this essential interface. For the surface a distorted bulk truncated termination and the sub-surface cation vacancy reconstruction model are used. The adsorption configuration space is sampled and configurations as input for DFT calculations are selected using unsupervised machine learning approaches. Structural, energetic, electronic, and vibrational results are presented and compared to carboxylic acids. Potentials for multi-scale modeling approaches are sketched.

O 81.2 Thu 15:15 CHE 91

Predicting platinum adatom geometries on hematite for single-atom catalysis — •Florian Buchner, Ralf Wanzenböck, Jesús Carrete, and Georg K. H. Madsen — Institute of Materials Chemistry, TU Wien, 1060 Vienna, Austria

In single-atom catalysis, where isolated adatoms anchored on a support are used as catalysts, performance is highly sensitive to the charge state and coordination of the adatoms. This offers new avenues to design and tune catalysts. But to do so efficiently, a detailed understanding of the potential energy surface (PES) of the adatom-substrate system is needed.

In this theoretical study, we present an application of an evolutionary algorithm, the covariance matrix adaptation evolution strategy (CMA-ES) [M. Arrigoni *et al.*, npj Comput Mater 7, 1–13 (2021)], to the prediction of Pt adatom configurations on the $(1\bar{1}02)$ surface of hematite (α-Fe_2O_3).

We find a rich PES that is not only governed by the large-scale adatom geometry but also reflects competing electron localization between the Pt and substrate Fe atoms, giving rise to sets of geometrically almost identical structures whose energies nonetheless span an appreciable range. We further discuss the effect of substrate doping on this localization and argue that a combination of different experimental methods and theory is required to understand observed adatom geometries.

O 81.3 Thu 15:30 CHE 91

Growth and adsorption studies of magnetite nanoparticles on Al2O3 — •Mohammad Ebrahim Haji Naghi Tehrani[1,2], Marcus Creutzburg[1], Heshmat Noei[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron (DESY), D-22603 Hamburg, Germany — [2]Fachbereich Physik Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany

Magnetite (Fe3O4) is an important transition metal oxide with diverse applications in catalysis, data storage and biomedical imaging. In this study, we grow model catalyst magnetite nanoparticles on Al2O3(0001) surface under UHV conditions and at different temperatures: 150, 300, 500, and 700°C. Grazing incidence X-ray diffraction (GIXRD) and microscopy techniques were assisted in defining the facet and morphology of the developed nanoparticles, respectively. GIXRD outcomes indicated the formation of 111 oriented nanoparticles. Fourier transmission infrared reflection-absorption spectroscopy (FTIRRAS) was performed to study the adsorption of formic acid on magnetite/Al2O3 samples. The results demonstrate different types of adsorption and dissociation of formic acid. The results of this study can be applied as a paradigm in order to provide insight into the fundamental surface science of the next generation of the hierarchical organic-linked magnetite.

O 81.4 Thu 15:45 CHE 91

Fe_3O_4(111): surface structure and CO adsorption — •Johanna Hütner[1], Florian Kraushofer[1], Matthias Meier[1,2], Zdenek Jakub[3], Cesare Franchini[2,4], Michael Schmid[1], Ulrike Diebold[1], Gareth S. Parkinson[1], and Jan Balajka[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Computational Materials Physics, University of Vienna, Austria — [3]CEITEC, Brno University of Technology, Czech Republic — [4]Department of Physics and Astronomy, Università di Bologna, Italy

The surface structure of Fe_3O_4(111) has been the subject of an ongoing debate. The most stable termination, over a wide range of oxygen chemical potentials, has a layer of tetrahedrally coordinated iron atoms (Fe_{tet1}). We present AFM data that show an almost perfect grid of

Fe_{tet1} atoms. In filled states STM images, iron atoms exhibit varying contrast, suggesting electronic structure variations among the cation sites. We study the adsorption of CO as a probe molecule on the $Fe_3O_4(111)$ surface with noncontact AFM. The data show that CO adsorbs on top of Fe_{tet1} atoms at all coverages. We identify coverage-dependent adsorption structures with varying CO–CO spacings. We propose that the apparent CO–CO repulsion is a substrate-mediated effect that could be explained by charge redistribution in the surface. The CO ordering on a defect-free $Fe_3O_4(111)$ surface is consistent with previously measured temperature programmed desorption data. Our findings contribute to the understanding of the electronic structure of the $Fe_3O_4(111)$ surface and will be a requisite for modeling the adsorption of more complex molecules.

O 81.5 Thu 16:00 CHE 91

Reactivity and Influence of Catalytic Support Materials - a combined in situ and operando Infrared Study of CeO2 — •Eric Sauter[1], Lachlan Caulfield[1], Alexei Nefedov[1], Florian Maurer[2], Daria Gashnikovina[2], Jan-Dirk Grunwaldt[2], and Christoph Wöll[1] — [1]Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), Engesserstraße 20, 76131 Karlsruhe, Germany

For most catalytic reactions the morphology, oxidation state and support were found to have a strong influence on the catalytic activity. Investigation of the most active sites, the support material and its behavior under model as well as realistic conditions is a prerequisite for a comprehensive understanding of catalytic processes. With Infrared Spectroscopy the surface composition and interaction with water, as well as carbon monoxide, can be investigated. The combination of low temperature, UHV gas adsorption as well as operando DRIFTS was used to characterize CeO2 as catalytic support material. The adsorption of CO on single crystals was used as reference for the interpretation of more complicated spectra like powders or nanoparticles. The interactions with water have shown the high reactivity of the cerium oxide surface, which at the end leads to hydroxyl termination. With the use of in situ and operando Infrared spectroscopy the behavior of catalysts and their support material can be investigated, under realistic reaction conditions, into more detail.

O 81.6 Thu 16:15 CHE 91

Reduction of ceria with carbon monoxide - A high resolution, operando DRIFTS study — •Lachlan Caulfield, Eric Sauter, and Christoph Wöll — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, 76344, Germany

In the last decades, ceria-based systems have seen an increase in popularity, due to its unique redox behavior and catalytic characteristics. Ceria powders are widely used in exhaust catalysts as well as other catalytic cycles, in particular due to the cheap and simple preparation methods. To gain a better understanding of the chemical and structural behavior of ceria nanoparticles and their interaction with gaseous molecules, an operando DRIFTS study was carried out. Following the complete oxidation of the powder samples, they were introduced in a carbon monoxide atmosphere at room temperature. By tuning the pressure of carbon monoxide gas as well as the reaction temperature inside the catalytic cell it was possible to observe the reduction and structural changes of ceria, induced by the presence of carbon monoxide. Using operando DRIFTS with carbon monoxide as a reducing agent as well as a probe molecule, the chemical and structural changes of ceria can be easily investigated.

O 81.7 Thu 16:30 CHE 91

Tailoring photolytic reaction products by application of a low interacting rare gas decoupling layer — •Inga Langguth[1], Julien Rowen[2], Wolfram Sander[2], and Karina Morgenstern[1] — [1]Chair of Physical Chemistry I, Ruhr-Universität Bochum, Germany — [2]Chair of Organic Chemistry II, Ruhr-Universität Bochum, Germany

While carbene molecules are known to be highly reactive and short living reactants in gas phase, they are passivated on metal surfaces upon chemisorption. Thin solid rare gas films on coinage metal surfaces are a novel type of decoupling layer applicable for STM investigations. Thus, it is taken advantage of the low interacting chemical environment of xenon (Xe) monolayer on Ag(110) in order to investigate the photolytic reactions of classical carbenes. The reaction products of the carbene coupling formed on the Xe layer adsorbed on the metal are straightforwardly accessed by subsequent Xe desorption. Vast structural differences reveal that the reaction products formed on the Xe substantially differ from the species formed under the same conditions on the metal surface. Both reaction products are compared, revealing the tool function of the non-ionic, low interacting rare gas decoupling layer for tailoring reaction pathways.

O 81.8 Thu 16:45 CHE 91

Methanol and water compete for the same adsorption sites on $In_2O_3(111)$ — Chiara Wagner[1], Andreas Ziegler[2], Michael Schmid[1], Bernd Meyer[2], Ulrike Diebold[1], and •Margareta Wagner[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Indium oxide, a transparent conductive oxide, has been discovered to be a highly selective catalyst for methanol synthesis by CO_2 hydrogenation. The large surface unit cell of $In_2O_3(111)$ exhibits a variety of Lewis acid and base sites for methanol and water adsorption. We compare the adsorption of both molecules under UHV conditions by employing AFM, STM, XPS, and TPD, together with DFT calculations. For medium coverages up to 9 molecules per surface unit cell we find a similar behavior: Initially, at room temperature, both molecules dissociate and protonate the most reactive O sites of the unit cell. When both molecules are dosed consecutively, methanol readily replaces water, while water is less efficient to substitute methanol. Below 300 K, both methanol and water adsorb molecularly in less-favored regions of the unit cell, still occupying the same sites and thus forming the same structural motifs. However, at coverages beyond 9 molecules per unit cell significant difference are found due to the ability of water to form and receive two hydrogen bonds instead of only one in the case of methanol.

O 81.9 Thu 17:00 CHE 91

How the (2x1) Reconstruction of Calcite (10.4) dominates the Desorption Kinetics of Water and Ethanol — •Tobias Dickbreder[1], Dirk Lautner[2], Antonia Köhler[1], Lea Klausfering[1], Ralf Bechstein[1], and Angelika Kühnle[1] — [1]Physical Chemistry I, Bielefeld University, 33615 Bielefeld, Germany. — [2]Institute of Physical Chemistry, Johannes Gutenberg University Mainz, Duesbergweg 10-14, 55099 Mainz, Germany.

Calcite, the most abundant carbonate mineral in the Earth's crust, plays a dominate role in a variety of environmental processes. Upon cleavage, calcite exposes the (10.4) cleavage plane with a rectangular unit cell. Interestingly, several experiments have been presented that suggest a (2x1) surface reconstruction. However, clear experimental evidence and a theoretical confirmation were long missing. Recently, an atomic force microscopy study provided convincing experimental indication for a (2x1) reconstruction at 5 K. Nevertheless, it remained unclear how the (2x1) reconstruction effects the surface properties of calcite. Here, we present temperature-programmed desorption (TPD) curves of water and ethanol desorbing from calcite (10.4) around room temperature. Our experiments can be excellently described by a kinetic model considering two different adsorption positions, as would be present in case of a (2x1) reconstruction. This finding applies to the desorption of water and ethanol, suggesting that the effect is not molecule specific, but characteristic for the calcite cleavage plane. Our results, thus, demonstrate that the (2x1) reconstruction has significant impact on the interfacial properties of calcite.

O 81.10 Thu 17:15 CHE 91

Identification of Intermediates in the Reaction Pathway of SO2 on the CaO surface: From Physisorption to Sulfite to Sulfate — •Nils Schewe[1], Farahnaz Maleki[2], Giovanni Di Liberto[2], Hicham Idriss[1], Gianfranco Pacchioni[2], and Christoph Wöll[1] — [1]Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, 76344, Germany — [2]Department of Materials Science, University of Milano-Bicocca, 20125 Milano, Italy

We report on the results of a combined experimental and theoretical study of the interaction of sulfur dioxide with a calcium oxide single crystal surface. Our investigation of this model system for flue gas desulfurization was carried out on the CaO (001) surface under ultra-high-vacuum conditions. Combining UHV infrared reflection absorption spectroscopy (IRRAS) with x-ray photo electron spectroscopy (XPS) and ab initio density functional theory (DFT) calculations, we were able to identify a three-step reaction path way. After the physisorption of SO2 at temperatures below 70 K on the ubiquitously hydroxylated surface, increasing the temperature leads to insertion of the SO2 into surface hydroxyl groups. Around 110 K the first insertion leads to a surface hydrogen-sulfite, which evolves into a surface hydrogen-sulfate with the second insertion into another OH-group above 160 K. The surface state was confirmed by DFT, where the predicted IR vibrational frequencies align with the experimentally observed ones.

O 81.11 Thu 17:30 CHE 91

Interaction and structural behavior of thymidine on polycrystalline cerium oxide films — •Sascha Mehl[1], Anastasiia Deineko[2], Viacheslav Kalinovych[2], Tomáš Skála[2], Iva Matolinová[2], Vladimír Matolín[2], Kevin C. Prince[1], and Nataliya Tsud[2] — [1]Elettra-Sincrotrone Trieste S.C.p.A., in Area Science Park, Strada Statale 14, km 163.5, Basovizza (Trieste), 34149, Italy — [2]Charles University, Faculty of Mathematics and Physics, Department of Surface and Plasma Science, V Holešovičkách 2, Prague, 18000, Czech Republic

Thymidine (dT) is a nucleoside and therefore important for the contribution to in-depth studies of cerium oxide as a potential sensing material applicable for analytes such as DNA. This topic contributes to a survey which embraces from simple nucleobases to more complex DNA components as probe molecules on a wide array of different CeO2 films. Consequently, bridging the material gap and deposition of dT from aqueous solution on compact CeO2 allows us to get closer towards more realistic conditions. The goals of the present study were the elucidation of the electronic structure of the biomolecule-cerium oxide interface, as well as the adsorption geometry and thermal stability of the nucleoside. Adsorption studies were carried out by using SRPES, RPES and NEXAFS techniques. A noteworthy result was the successful deposition of dT from solution and in gas phase without decomposition, which was never previously reported in the literature. The analysis of the experimental data revealed that dT molecules anchor on CeO2 film via two carbonyl oxygen atoms and an amino group.

O 81.12 Thu 17:45 CHE 91

Modeling Bio-MOFs for Anesthetic Xenon Recovery: The Role of Noncovalent Host-Guest Interactions — •Yeliz Gurdal — Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany — Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany — Department of Bioengineering, Adana Alparslan Türkeş Science and Technology University, 01250 Adana, Türkiye

Taking advantage of metal organic frameworks (MOFs) for anesthetic Xe recovery has been a recent topic studied rarely in the literature. In this work, Xe recovery performances of 43 biological MOFs (Bio-MOFs) consisting of biocompatible cations and linkers have been studied by means of Grand Canonical Monte Carlo, Density Functional Theory, and Molecular Dynamics simulations. Results reveal that Xe-host interactions are maximized mainly due to noncovalent interactions of Xe, such as charge-induced dipole and aerogen-π interactions. Polarized Xe atoms in the vicinity of cations/anions as well as π systems suggest enhanced guest-host interactions. The results of this work depict examples of superficially studied aerogen interactions playing an important role in selective adsorption of Xe in porous materials. This study has received funding from the TUBITAK under the 1002 Short Term R&D Funding Program (grant agreement No: 120Z160).

O 82: Graphene I: Adsorption, Intercalation and Doping

Time: Thursday 15:00–17:15 Location: GER 37

O 82.1 Thu 15:00 GER 37

Graphene quantum dot nanoarray in a van der Waals heterostructure — •Keda Jin[1,2,3], Junting Zhao[1,2,3], Tobias Wichmann[1,3,4], F. Stefan Tautz[1,3,4], Jose Martinez-Castro[1,3], Markus Ternes[1,2,3], and Felix Lüpke[1,3] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany. — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany. — [3]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Jülich, Germany. — [4]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany.

Graphene quantum dots (GQDs) are promising candidates for spin qubits because of their long spin coherence and short switching time. Although isolated GQDs have been created in van der Waals (vdW) heterostructures, the fabrication of GQD nanoarrays is still an ongoing challenge. Here, we realize a regular two-dimensional array of GQDs in a vdW heterostructure composed of graphene on a single layer of 1T-NbSe$_2$ on top of 2H-NbSe$_2$ (Gr/1T/2H-NbSe$_2$) by combining mechanically assembled vdW heterostructures and nanoscale phase engineering. Using scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM), we demonstrate that the 1T-NbSe$_2$ phase periodically dopes the graphene layer, which in response exhibits quantized charge states that can be manipulated by the local electric field of the tip. Our findings show a possible route for the creation of a highly dense GQD nanoarray with a potential application in the quantum technologies.

O 82.2 Thu 15:15 GER 37

Sn-induced superstructures at the EG/SiC(0001) interface and their influence on EG — •Zamin Mamiyev, Chitran Ghosal, and Christoph Tegenkamp — Institut für Physik, Technische Universität Chemnitz

Intercalating chemical elements into the buffer layer/SiC(0001) interface is a promising approach to delaminate a single carbon layer forming extended epitaxial graphene (EG) layers with new properties. In this regard, Sn is an interesting candidate because the triangular monolayer structure on SiC(0001) was shown to exhibit a Mott state [1].

By means of low energy electron diffraction we studied recently in detail the intercalation of Sn below the buffer layer grown before on SiC(0001) and found 1×1 and $(\sqrt{3}\times\sqrt{3})$ Sn induced phases depending on details of the annealing procedure [2]. As deduced from transport but also local spectroscopy, the former is metallic while the latter reveals a band gap opening. In addition, we found a $(\sqrt{3}\times\sqrt{3})$R30° interference pattern with respect to the EG lattice. This so-called broken Kekulé order forms due to the breaking of the bond order in EG and often found in the vicinity of buckled Sn(1×1) subsurface clusters opening the channel for K,K' scattering in EG. The electronic structure and, in particular, the formation of a Mott gap will be investigated by electron energy loss spectroscopy.

[1] S. Glass et al., PRL 114, 247602 (2015). [2] Z. Mamiyev and C. Tegenkamp, Surf. & Int. 34, 102304 (2022).

O 82.3 Thu 15:30 GER 37

Stabilizing high-overlap organic crystals by n-doped graphene — •Fabio Calcinelli and Oliver Hofmann — Graz University of Technology, Graz, Austria

Organic thin-films are known for their tuneable properties, which are strongly dependent on the polymorph the films assume. Traditional ab-initio studies of thin films geometries remain computationally prohibitive, due to the immense number of possible configurations, and this results in the need for structure-property relationships to help in the design of materials with certain target properties.

In this contribution, we examine the correlation between the energy of polymorphs and their interlayer LUMO-LUMO overlap for benzoquinone on n-doped graphene. Employing smart-data machine learning, we use a small number of DFT calculations to predict the energy and the LUMO-LUMO overlap for a large sample of polymorphs. We assess the impact of the n-doping of the substrate on this overlap/stability relationship by performing the energy and overlap evaluation for different intensities of n-doping.

We find that, for low dopant concentrations, there exists no relationship between interlayer overlap and stability, while for high dopant concentrations, it appears that polymorphs with high LUMO-LUMO overlap are predominant in the stability ranking. We explain this different behavior as the consequence of charge transfer from the substrate to the first molecular layer producing different LUMO occupations for different dopant concentrations, resulting in a stabilizing effect of high LUMO-LUMO overlap for high concentrations only.

O 82.4 Thu 15:45 GER 37

Theoretical studies of nitrogen-doped corrugated graphene on metal supports — •Ivan Abilio[1] and Krisztián Palotás[1,2] — [1]Wigner Research Center for Physics, Budapest, Hungary — [2]ELKH-SZTE Reaction Kinetics and Surface Chemistry Research Group, Szeged, Hungary

For maximizing the usability of N-doped graphene materials, the microscopic understanding of their structures (graphitic, pyridinic, pyrrolic, etc) and electronic properties at the atomic scale is crucial. Motivated by this, density functional theory calculations of N-doping configurations in corrugated graphene single layers on Ir(111) and Ru(0001) substrates were performed. Taking systematically selected N-doped graphene defect configurations, their energetic preference is found to be correlated with their atomic structure. Scanning tunneling microscopy simulations with different tip models [1] were performed, and a great variety of STM image contrasts showed a good agreement with experimental STM images. The negatively charged N atoms embedded into the corrugated graphene layer suggest single atom catalytic potential for these structures.

Financial support from NKFI OTKA 124100 & 138714, the János Bolyai Research Grant of the Hungarian Academy of Sciences (BO/292/21/11), the New National Excellence Program of the Ministry for Culture and Innovation from NKFI Fund (ÚNKP-22-5-BME-282) and the Stipendium Hungaricum Scholarship is gratefully acknowledged.

[1] G. Mándi and K. Palotás, Phys. Rev. B 91, 165406 (2015).

O 82.5 Thu 16:00 GER 37

Formation model of AlF$_3$ intercalated aggregates on HOPG surfaces for rechargeable battery applications — •Sindy Rodríguez Sotelo[1,2], Adriana Candia[1], Igor Stanković[3], Mario Passeggi Jr.[1,2], and Gustavo Ruano[4] — [1]IFIS, CONICET-UNL, Santa Fe, Argentina — [2]FIQ, UNL, Santa Fe, Argentina — [3]Scientific Computing Laboratory, Center for the Study of Complex Systems, IPB, Belgrade, Serbia — [4]CAB, CNEA, Bariloche, Argentina

Rechargeable batteries based on ion intercalation are currently of great interest, with lithium being the most studied and with the best performance. However, the limited reserves of this material and its scarce distribution in the world have led to the research for new alternatives. In our recent work, we studied the intercalation of AlF$_3$ in HOPG as a new possibility to use this molecule in rechargeable batteries and to understand its role when used as a solvent component [1,2]. Based on our recent reports, in this work we theoretically and experimentally characterize the dynamics of the AlF$_3$ interlayers, to discuss the possibility of decoupling the first graphene layers from the HOPG under ultra-high vacuum conditions. We show experimental measurements performed by STM, XPS and AES, also proposing a model to glimpse the growth and behavior of AlF$_3$ in the surface layers of the HOPG substrate, to provide clarity regarding the formation of the AlF$_3$/HOPG interface. We complement the analysis with calculations in the formalism of DFT and molecular dynamics (MD). **References** [1] A.E. Candia *et al.* Carbon, 186 (2022) 724. [2] Rodríguez *et al.* Phys. Chem. Chem. Phys, 23 (2021), 19579.

O 82.6 Thu 16:15 GER 37

Atomic and electronic structure of intercalated Pb layers in proximity to epitaxial graphene — •Chitran Ghosal, Markus Gruschwitz, Julian Koch, and Christoph Tegenkamp — Institut für Physik, TU Chemnitz, Chemnitz, Germany

Selective intercalation into the buffer layer/SiC(0001) interface can realize atomically sharp interface layers near epitaxial graphene that resemble novel 2D heterosystems. High-Z elements are interesting candidates, not only because they are expected to host Dirac fermions, but also because spin effects are expected in graphene.

Intercalation of Pb leads to the formation of different phases, which we have studied in detail using scanning tunneling microscopy. As recently shown, intercalated Pb bilayers form nanostripes under graphene and show fingerprints of plumbene. These Pb layers are rotated with respect to graphene, which breaks the sublattice symmetry and is associated with an electronic gap in graphene [1]. Hexagonally arranged bubble-like structures with an average size of 2.3 nm were also found. Scanning tunneling spectroscopy (STS) again revealed the formation of mini-gaps in the 2D heterosystem. Spatially resolved mapping of the electronic structure also clearly showed the existence of a network of edge states around the edges of the bubbles.

[1] C. Ghosal et al., PRL 129, 116802 (2022)

O 82.7 Thu 16:30 GER 37

Tailoring permanent carrier density in epitaxial graphene by F4-TCNQ molecular doping for quantum Hall resistance standards — •Yefei Yin, Atasi Chatterjee, Davood Momeni, Mattias Kruskopf, Martin Götz, Stefan Wundrack, Frank Hohls, Klaus Pierz, and Hans Werner Schumacher — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

A prerequisite for the development of graphene electronics is the reliable control of its carrier density. Since epi-graphene on SiC already exhibits a high electron density of up 10^{13} cm^{-2}, the goal is a controlled reduction towards the charge-neutrality point. This was achieved by molecular doping with the acceptor F4-TCNQ doping stacks deposited on graphene. By precise adjustment of the dopant concentration and controlling the initial carrier density of the undoped graphene, we can tune the carrier density in a wide range from intrinsic n- to the p-type. Precision measurements of the quantum Hall resistance show a quantization accuracy of 10^{-9} which underlines the high quality and suitability of this doping method for electronic device application in metrology. [1] Our data show a correlation between the electron density and the onset of the i = 2 quantum Hall plateau which gives a valuable criterion for evaluating graphene-based resistance standards since the *classical* relation (n = ieB/h) to determine the centre of the quantum Hall plateau is not valid in epi-graphene. The results are discussed in the charge transfer model. [1] Y.Yin et al., Adv. Physics Res. 2022, DOI: 10.1002/apxr.202200015.

O 82.8 Thu 16:45 GER 37

Transport properties of intercalated epitaxial graphene — •Markus Gruschwitz, Zamin Mamiyev, Chitran Ghosal, Susanne Wolff, Thomas Seyller, and Christoph Tegenkamp — Institut für Physik, TU Chemnitz, Chemnitz, Germany

Large-scale growth and electronic manipulation of graphene are of great interest for nanoelectronics applications. The former is already realized by epitaxial growth and intercalation of buffer layers on SiC(0001). Electronic properties such as doping level and gap opening of the decoupled graphene layer strongly depend on the element and the structure of the interface. In this study we investigated Sn, Bi and In intercalated graphene by means of nanoscopic transport, supplemented by STM, LEED and PES. Depending on the film thickness and temperature, (1x1) phases can be formed with all three elements, accompanied by the formation of free-standing graphene. The fully intercalated phases show metallic conductivity behavior ($\sigma_{\mathrm{Sn}}=0.63\,\mathrm{mS}/\square$, $\sigma_{\mathrm{Bi}}=0.74\,\mathrm{mS}/\square$). The slightly lower conductivity of 10% compared to clean MLG is most likely due to interface scattering rather than different doping levels of the EG. Further heating allows the formation of $\sqrt{3}$-structures for all intercalants. Thereby, the conductivities drop by 2-3 orders of magnitude, accompanied by an increase of the anisotropy with respect to SiC step structure. This is indicative of inhomogeneous desorption especially around the step edges. The detailed analysis with the variable range hopping model yield localization lengths that correlate with the size of intercalated areas.

O 82.9 Thu 17:00 GER 37

Magnetotransport and structural properties of Bi(110) islands on epitaxial graphene — •Julian Koch[1], Sergii Sologub[1,2], Chitran Ghosal[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

Magnetotransport measurements at 10 K using a 4 T magnet were performed on Bi islands on monolayer graphene/SiC with average thickness up to 3.6 bilayers (BL). They are supported by structural investigations using SPA-LEED and STM, which reveal that Bi predominately grows as needle-like islands with a (110) termination.

The analysis of the magneto and Hall conductivity gives the electron concentration and the mobility. The electron concentration slightly decreases with $4\cdot10^{11}$ cm^{-2}BL^{-1} from an initial value of $1.4\cdot10^{13}$ cm^{-2} for the clean surface. The mobility decreases from 2100 cm^{2}V^{-1}s^{-1} to a minimal value of 1630 cm^{2}V^{-1}s^{-1} at 2.4 BL. Moreover, the electron electron interaction contribution to the magneto conductivity, which is almost negligible for the clean surface, strongly increases linearly with approximately 0.44 mS/BL. At 3.6 BL it is equal to approximately half the Drude conductivity at zero field.

The weak localization (WL) of the clean surface gradually transitions to weak anti-localization (WAL) with increasing Bi coverage. This is associated with a decrease of the dephasing length of the scattered electrons, which is correlated with the average distance of the islands obtained from STM measurements.

O 83: Focus Session: Ultrafast Dynamics in Nanostructures II

Time: Thursday 15:00–17:30 Location: GER 38

Topical Talk O 83.1 Thu 15:00 GER 38

Imaging ultrafast electron dynamics in isolated nanoparticles — •Daniela Rupp — LFKP, ETH Zurich, Switzerland

Atomic clusters and nanodroplets are used as ideal model systems over all wavelength regimes for exploring the ultrafast physical processes underlying the formation and evolution of highly excited matter. Via single-pulse single-particle coherent diffractive imaging (CDI) with the intense femtosecond pulses from short-wavelength free electron lasers (X-FELs), it became possible to study single specimen in free flight.

In CDI, the elastically scattered light forms an interference pattern that encodes the particle's structure, allowing to investigate the morphology of fragile and short-lived specimen. Also light-induced dynamics after pulsed laser excitation can be visualized by time-resolved CDI. Even changes in the electronic properties were found to be imprinted in the CDI patterns, but their time-evolution could not be investigated with typical pulse durations of 100 femtoseconds.

We recently showed that, under favorable conditions, single helium nanodroplets can be also imaged with an intense HHG source, providing much shorter pulses. In time-resolved experiments, a moderately intense near-infrared (NIR) laser pulse, too weak to ionize helium nanodroplets, dramatically changed their scattering response in the extreme ultraviolet (XUV) regime. The ability to switch the optical properties of nanoscale matter within less than a femtosecond, and observe this temporally and spatially resolved, promise to impact a broad field of science from non-linear XUV optics to ultrafast material science.

O 83.2 Thu 15:30 GER 38

Sub-picosend Elastic Response of a supported Pd Nanoparticle Ensemble studied by Time-resolved X-ray Diffraction — Simon Chung[1], Thorben Eggert[2], •Vedran Vonk[1], Nastasia Mukharamova[1], Sebastian Matera[2], Roman Shayduk[3], Johannes Moeller[3], Nils Schewe[4], Eric Sauter[4], Christoph Schreuer[2], Anders Madsen[3], Karsten Reuter[2], and Andreas Stierle[1] — [1]CXNS - Centre for X-ray and Nanoscience, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6t, Berlin, 10587, Germany. — [3]European X-Ray Free-Electron Laser Facility GmbH, Holzkoppel 4, Schenefeld, 22869, Germany. — [4]Institute of Functional Interfaces (IFG), Karlsruher Institut fur Technologie (KIT), Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, 76344, Germany.

We report on the results of a combined experimental and theoretical study of the structural response of a Pd nanoparticle ensemble upon fs-laser excitation. Time-resolved X-ray diffraction experiments, having a time resolution of approx. 100 fs, were performed at end-station MID of the European X-ray Free Electron Laser (XFEL). Molecular dynamics simulations were done taking explicitly into account the particle size distribution, as determined from SEM. The results are interepreted in terms of the dephasing of size-dependent elastic modes and picosecond energy dissipation of the nanoparticle ensemble towards the MgO single crystal support. An overview will be given about the experimental details, data analysis and molecular dynamics simulations.

O 83.3 Thu 15:45 GER 38

Description of High Garmonic Generation in Quantum Dots using a Tight-Binding approach — •Martin Thümmler[1], Alexander Croy[1], Stefanie Gräfe[1], and Ulf Peschel[2] — [1]Institute of Physical Chemistry, University of Jena — [2]Institute of Condensed Matter Theory and Optics, University of Jena

Recently, high harmonic generation (HHG) was experimentally observed in quantum dots showing striking differences compared to HHG in molecules and bulk materials. At the same time, the available theoretical tools (like semiconductor Bloch-equations and real-time density-functional theory (DFT)) have proven to be insufficient to describe the size dependence of the nonlinear response of these nanostructures. Here, we present a computationally feasible, real-space tight-binding method to account for the description of inter- and intraband harmonics, and ionization effects, while all model parameters are derived from DFT calculations. Inspired by recent experiments, we present first simulation results of HHG in 3D CdSe quantum dots for linear and elliptic polarization of the driving laser.

O 83.4 Thu 16:00 GER 38

Imaging of femtosecond spin dynamics at the nanoscale — •Sergey Zayko[1,4], Hung-Tzu Chang[1], Ofer Kfir[2], Timo Schmidt[3], Jakob Hagen[1], Michael Heigl[3], Murat Sivis[1,4], Manfred Albrecht[3], and Claus Ropers[1,4] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]School of Electrical Engineering, Tel Aviv University, Tel Aviv, Israel — [3]Experimental Physics IV, Institute for Physics, University of Augsburg, Germany — [4]IV Physical Institute, Solids and Nanostructures, Georg-August University

Femtosecond pulse durations combined with broad extreme-UV spectrum inherent to high harmonic generation (HHG) grant spectroscopic access to various material properties and phenomena including charge, spin and lattice dynamics. Here, we extend the applicability of HHG sources to direct real-space imaging of ultrafast processes. Specifically, we map femtosecond spin dynamics induces by optical excitations ferro- and ferrimagnetic materials. Our results demonstrate the first implementation of HHG radiation for element specific imaging as well as the first real-space imaging of femtosecond dynamics. Moreover, the achieved spatio-temporal resolution (down to 13.5 nm spatial and 15 fs temporal) is more than an order of magnitude higher than any magneto-optical imaging scheme reported so far, which would facilitate deeper fundamental understanding and, in particular, support application-oriented studies. Notably, the developed imaging scheme is directly applicable to a broad range of phenomena including transient absorption and structural phase transitions.

Topical Talk O 83.5 Thu 16:15 GER 38

Ultrafast coherent manipulation of free electrons via quantum interaction with shaped optical fields — •Giovanni Maria Vanacore — Department of Materials Science, University of Milano-Bicocca, Via Cozzi 55, 20126 Milano

The interaction between light and electrons can be exploited for generating radiation, or for controlling electron beams for dynamical investigation of materials, enabling new applications in quantum technologies and microscopy. In this contribution, I will describe an innovative method for coherent and versatile longitudinal/transverse manipulation of a free-electron wave function. Using appropriately shaped light fields in space and time, I will demonstrate how to modulate the energy, linear and orbital angular momenta, as well as spatial and temporal distributions of the electron wave function. The experiments have been performed in an ultrafast-TEM, where a pulsed electron beam was made to interact with shaped optical field generated via a spatial light modulator. The energy-momentum exchange resulting from such interaction was directly mapped via momentum-resolved ultrafast electron energy-loss spectroscopy. Our approach for arbitrary longitudinal/transverse electron modulation at the sub-fs timescale would pave the way to achieve unprecedented insights into non-equilibrium phenomena in advanced quantum materials, playing a decisive role in the rational design and engineering of future photonics and electronics application.

Funding source: SMART-electron project that has received funding from the EU Horizon 2020 Programme under GA No 964591.

O 83.6 Thu 16:45 GER 38

Structural Dynamics in Nanostructured Systems Probed by Ultrafast Transmission Electron Microscopy — •Nora Bach[1], Armin Feist[2], Marcel Möller[2], Claus Ropers[2], and Sascha Schäfer[1] — [1]Institute of Physics, University of Oldenburg, Germany — [2]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

One successful approach to investigate ultrafast nanoscale structural dynamics and to disentangle different excitation mechanisms in spatially inhomogeneous systems is based on local diffractive probing with nano-focused femtosecond electron pulses in an ultrafast transmission electron microscope (UTEM). Employing the Göttingen UTEM [1,2] in ultrafast convergent electron beam diffraction (U-CBED) mode [3], we study local dynamics in a multi-component model system consisting of a metal/semiconductor hybrid structure. Ultrashort optical excitation of a platinum stripe on a silicon membrane results in the generation of a multi-modal distortion wave propagating through the membrane. Pronounced lattice distortions are quantitatively tracked by U-CBED, and experimental results are reproduced by numerical simulations demonstrating that a superposition of Lamb waves at resonance frequencies of the bilayer structure [4] governs the evolution of the displacement inhomogeneity within the depth of the membrane.

[1] A. Feist, N. Bach, et al., Ultramicroscopy 176, 63 (2017).
[2] N. Bach et al., Struct. Dynamics 6, 014301 (2019).
[3] A. Feist et al., Struct. Dynamics 5, 014302 (2018).
[4] N. Bach et al., Struct. Dynamics 8, 035101 (2021).

O 83.7 Thu 17:00 GER 38

Controlling and shaping the electron recoil and energy transfer via nearfield geometry — •Fatemeh Chahshouri[1] and Nahid Talebi[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel, Nano, Surface, and Interface Science, KiNSIS, Kiel University, 24098 Kiel, Germany

Inelastic interaction of free-electrons with optical near fields has recently attracted attention for manipulating and shaping free-electron wave packets. Understanding the nature and the dependence of the inelastic cross section on the polarization of the optical near-field modes of the nanostructures is important for both fundamental studies and the development of new applications in this field. Here, we investigate the effect of the laser-field polarization and nanostructures asymmetric geometry on shaping free-electrons and controlling the energy transfer mechanisms, but also tailoring the electron recoil. We show that, an oblique incident electric field improves the coupling efficiency for coherent control of the longitudinal and transversal phase modulation of an electron wave packet. We also demonstrate the possibility of tailoring the shape of the localized plasmons by incorporating specific arrangements of nanorods to enhance or hamper the transversal and longitudinal recoils of free-electrons. Our findings open up a route towards the spatial characterization of plasmonic near-fields for the coherent manipulation and control of slow electron beams for creating desired shapes of electron wave packets.

O 83.8 Thu 17:15 GER 38

Light-induced hexatic state in a layered quantum material — •Till Domröse[1], Thomas Danz[1], Sophie F. Schaible[2], Kai Rossnagel[3,4], Sergey V. Yalunin[1], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisicpinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany — [3]Institute of Experimental and Applied Physics, Kiel University, Germany — [4]Ruprecht Haensel Laboratory, DESY, Hamburg, Germany

Ultrafast transmission electron microscopy (UTEM) is a powerful technique for resolving non-equilibrium dynamics on the nanoscale, employing a stroboscopic laser pump/electron probe approach [1]. Here, we harness the high-coherence electron source of the Göttingen UTEM [2] in the investigation of a structural phase transition between two charge-density wave (CDW) phases in a layered material [3]. A three-dimensional reconstruction of the nascent CDW order by means of ultrafast tilt-series nanobeam diffraction allows us to identify a transient hexatic state in the early stages of the phase formation. As the optical excitation induces a loss of interlayer correlations, this two-dimensional intermediate is characterized by a high density of topological defects suppressing the translational symmetry, while the orientational order is weakly preserved. On longer timescales, defect recombination and the establishment of the equilibrium stacking sequence lead to the formation of the long-range ordered high-temperature CDW phase.

[1] A. H. Zewail, Science **328**, 187-193 (2010).
[2] A. Feist *et al.*, Ultramicroscopy **176**, 63-73 (2017).
[3] T. Domröse *et al.*, in Review, arXiv:2207.05571 [cond-mat.mtrl-sci]

O 84: Focus Session: Making Experimental Data F.A.I.R. – New Concepts for Research Data Management I (joint session O/TT)

Data have been identified as major resource of the 21st century, unlocking great potential if refined and processed in the right way. In scientific research, particularly modern data science concepts like machine learning or neural networks enable novel types of data analysis with often strong predictive power. This Focus Session aims at providing a framwork for presenting and discussing novel concepts, tools and platforms for managing experimental research data related to surface science and solid-state physics. In particular, in light of the German NFDI initiative, where several consortia are actively working on tackling the imminent challenges of research data management in experimental solid-state physics, this Focus Session will offer an ideal environment for exchange among researchers, and bringing these novel developments into the labs. The intended topics include the description of experimental data and meta data generation workflows, meta data schemas and file formats, electronic lab notebooks, novel tools for handling and analyzing scientific research data, as well as sharing and searching platforms according to F.A.I.R. principles.

Organizers: Martin Aeschlimann (TU Kaiserslautern), Laurenz Rettig (FHI Berlin) and Heiko Weber (U Erlangen)

Time: Thursday 15:00–18:30 Location: WIL A317

Topical Talk O 84.1 Thu 15:00 WIL A317

Introducing a FAIR research data management infrastructure for experimental condensed matter physics data — •Christoph Koch — Humboldt-Universität zu Berlin, Department of Physics & IRIS Adlershof, Berlin, Germany

Digitization and an increase in complexity and price of experimental materials characterization techniques, an increase in accuracy and system size of computational solid state physics (or computational materials science), and the maturation of machine learning tools to extract patterns from large amounts of very diverse (annotated) data promise an acceleration of materials development by synergistically combining research data from many sources. While some labs start to upload their (raw) research data to data repositories, this is only a first but not sufficient step in leveraging the above-mentioned potential, since such repositories are typically either specific to a very particular technique or agnostic to the content of the data being uploaded. In both cases the research data cannot easily, and definitely not without significant human effort, be compared to and integrated with experimental data from other sources, or numerical predictions. In this talk I will report on recent progress of the FAIRmat NFDI consortium in extending the novel materials discovery laboratory (NOMAD), the world's largest data base for ab-initio computational materials data, to ingest experimental research data on the synthesis and characterization of materials in a machine-accessible manner, i.e. annotated with well-defined and interoperable metadata, achieved by establishing links between related (experimental and computational) quantities.

O 84.2 Thu 15:30 WIL A317

Introducing an electronic laboratory notebook in a col-

laborative research center — •Sebastian T. Weber[1], Aneta Daxinger[1], Philipp Pirro[1], Marek Smaga[1], Christiane Ziegler[1], Mathias Kläui[2], Georg von Freymann[1], Baerbel Rethfeld[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau — [2]Institute of Physics, Johannes Gutenberg University Mainz

The basis of a FAIR data management is a well-described and detailed documentation of every single step of the experiment and data analysis. In recent decades, however, the focus has shifted from analog measuring instruments and analytical calculations to computer-based experiments and simulations. This has lead to a large increase in the numbers of measurements and observed quantities and therefore in the amount of data generated. Consequently, traditional paper lab notebooks have reached their limits. Electronic lab notebooks (ELNs) are better suited for storing, indexing, searching and retrieving a large amount of entries. In particular, the automated filling-in of meta data can lead to a reduction in the workload of the scientists in the long term.

We present the lessons learned on challenges and advantages with the introduction of a joint electronic lab notebook within our collaborative research center CRC/TRR173 *Spin+X*. We report on our experiences in the daily work of the scientists and in education in student labs.

O 84.3 Thu 15:45 WIL A317

An efficient workflow for processing single event dataframes. — •Steinn Ýmir Ágústsson[1], M. Zain Sohail[2,3], David Doblas Jiménez[4], Dmytro Kutnyakhov[3], and Laurenz Rettig[5] — [1]Aarhus University, DK — [2]RWTH, Aachen — [3]DESY, Hamburg — [4]Eu-XFEL, Schenefeld — [5]FHI, Berlin

Single event resolved data streams measured by delay-line-detectors allow to correlate each measured photoelectron with the state of the experimental apparatus. This allows corrections and calibrations to be applied on a shot-to-shot basis and a flexible investigation of correlations between various measurement parameters.

We are developing an open-source python package[1], where highly optimized dataframe management and binning methods enable leveraging the full potential of event-resolved data structures. The flexible design of the pipeline allows processing any event-resolved data stream.

With momentum microscopy as the primary target application, we developed axis calibration and artifact correction methods designed to be agnostic to the experimental apparatus. These methods are tested on data generated by microscopes at FELs (HEXTOF@FLASH) as well as at HHG sources (FHI), but are easily exended to other endstations using similar detection techniques.

Our aim is to provide tools for the community which will reduce the development time for each end station, as well as an open and accessible data processing pipeline, built around the FAIR data principles.

[1] github.com/openCOMPES/sed

O 84.4 Thu 16:00 WIL A317

FAIR Data Infrastructure for Computation: Advanced many-body methods. — •José M. Pizarro[1], Nathan Daelman[1], Joseph F. Rudzinski[1,2], Luca M. Ghiringhelli[1], Roser Valentí[3], Silvana Botti[4], and Claudia Draxl[1] — [1]Institut für Physik und IRIS-Adlershof, Humboldt-Universität zu Berlin — [2]Max-Planck-Institut für Polymer Forschung, Mainz — [3]Institut für Theoretische Physik, Goethe University Frankfurt am Main — [4]Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena

Big-data analyses and machine-learning approaches have recently emerged as a new paradigm to study and predict properties of materials. In order to perform these analyses, materials data have to be structured in a FAIR (findable, accessible, interoperable, and reusable) format [1]. While most of the current databases deal with density-functional-theory (DFT) calculations, there is a clear need for developing FAIR-data schema for methodologies going beyond DFT. Methods such as the *GW* approximation, dynamical mean-field theory, and time-dependent DFT allow to calculate excited- and many-body-states properties beyond DFT, thus having a direct quantitative comparison with experiments. In this talk, we will introduce the achievements and challenges undertaken within the FAIRmat consortium towards fully structuring the (meta)data of all these techniques. We demonstrate how users can analyze the data and compare with angle-resolved photoemission spectroscopy.

[1] M. Scheffler et al., Nature **604**, 635 (2022).

O 84.5 Thu 16:15 WIL A317

Electronic Laboratory Notebooks for FAIR Data Management; Evaluation and Recommendations for Solutions at Research Infrastructures — •Philipp Jordt[1], Wiebke Lohstroh[2], and Bridget Murphy[1] — [1]IEAP, Kiel University, Germany — [2]MLZ, Technische Universität München, Germany

Electronic Laboratory Notebooks (ELN) are the digital counterpart to the classical handwritten paper notebook and play a vital role in the implementation of FAIR data standards. Modern ELN solutions range from simple note taking applications to integrated tools, combining documentation, inventory management, progress tracking and more. Nowadays, ELNs are becoming more prominent in research laboratories around the world, replacing paper notebooks. This evaluation of basic needs was carried out in the context of the DAPHNE4NFDI consortia. Of special interest is the view on ELNs for combined use at large scale facilities and in the home laboratory. Thus, the requirements regarding implementation, deployment, authentication, etc., may differ from those for single or laboratory use at universities. An overview of different concepts and existing solutions is given. Multiple ELNs have been evaluated during test runs at large scale facilities and a survey on existing solutions was held. From these results, a list of ELN specifications is presented, ranging from useful to necessary. These insights may serve as a guideline for evaluating or implementing ELNs in the future.

O 84.6 Thu 16:30 WIL A317

Ontology for Experimental Data — •Sandor Brockhauser — Center for Materials Science Data, Humboldt-Universität zu Berlin, Germany

Ontology is the scientific field of formal knowledge representation. This field contributes to Data Science and helps Experimentalist to properly annotate their data and metadata on a FAIR way. During the last decades several different ways have been developed in the field of Ontology for describing knowledge as a set of information and their relationships. These include Information mapping, Concept maps, Topic maps, Mind maps, Knowledge graphs, BORO (Business Objects Reference Ontology), RDF (Resource Description Framework), OWL (Web Ontology Language), ORO (Object-Role Modeling), UML (Unified Modeling Language), ISO 15926 (standard for data sharing), OLOG (mathematical framework for knowledge representation), GELLISH (ontology language for data storage and communication), etc. For describing experimental facts, we suggest using an ontology in OWL which is derived from the NeXus community standard. It represents all the concepts developed for explaining experiments and experimental data, just like the relationships between them. Such representation allows connecting the concepts defined in NeXus also to other ontologies. Additionally, any data management systems, like NOMAD which accepts experiment data provided in the NeXus standard, can immediately link the data and metadata to the ontology and make them interoperable.

15 min. break

Topical Talk O 84.7 Thu 17:00 WIL A317

Open Research Data for Photons and Neutrons: Applications in surface scattering and machine learning — •Linus Pithan — Universität Tübingen, Institut für Angewandte Physik - DAPHNE4NFDI

Open (F.A.I.R.) research data is becoming a key ingredient for data driven machine learning (ML) applications that requires access to existing data of preceding experiments - which goes well beyond data collected in the context of one's own experiments which one might keep in a secret drawer. We will discuss current possibilities as well as future opportunities and challenges with special emphasis on surface scattering. Embedded in the DAPHNE4NFDI (DAta from PHoton and Neutron Experiments) consortium we present efforts on how data catalogs may serve as backbone for F.A.I.R. datasets provided by synchrotron and neutron sources or through community efforts. Besides suitable metadata collection also the harmonization of data- and metadata formats are issues still to be tackled especially for systematic access to fully analyzed, experimental datasets (e.g. by adopting NeXus community conventions). After a broader overview and shining light on the SciCat meta-data catalog system,[1] we discuss as application examples efforts in the field of reflectometry (XRR, NR) [2,3] and X-Ray scattering and diffraction (WAXS, GIWAXS and XPCS).[1,4]

[1] V. Starostin, L. Pithan et al. 2022, SRN, Vol. 35, No. 4

[2] A. Greco et al. 2022, J. Appl. Cryst. 55 362

[3] L. Pithan et al., Refl. dataset, 10.5281/zenodo.6497438
[4] V. Starostin et al. 2022, npj Comp. Mat. 8, 101

O 84.8 Thu 17:30 WIL A317

NOMAD OASIS as a Tool for Electron and Atom Probe Microscopists — •Markus Kühbach — Department of Physics, Humboldt-Universität zu Berlin, Germany

Embracing the FAIR principles for sharing data and knowing how to work with different tools in research data management systems is becoming an invaluable skill in a scientist's daily life. Embracing such systems of tools, one of which is offered with NOMAD OASIS, allows you to start organizing your research data locally. Learning such tools will train you to understand what schemes and electronic lab notebooks are and how the data and metadata are processed by these tools. Example implementations of specific workflows can give you ideas where to start from and how to customize these tools for the needs of your own research and colleagues. Thereby, you can provide feedback which supports the evolution and improvement of the research data management system.

NOMAD OASIS offers you many examples which show now also how data and metadata of specific experiments can be parsed into a standardized representation. These examples teach users through detailing how data can be entered, viewed, and organized with customizable schemes in NOMAD. Furthermore, the examples suggest strategies for how the information in NOMAD can be accessed for generic or domain-specific data analytics tools.

In my talk, I will go through one or two of these examples specific to electron microscopy (orientation imaging microscopy or spectroscopy).

O 84.9 Thu 17:45 WIL A317

FAIR Data Infrastructure for Computation: Introducing the parsers for Quantum Monte Carlo and ALF — •Jonas Schwab[1], José M. Pizarro[2], Jefferson Stafusa E. Portela[1], Luca M. Ghiringhelli[2], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Institut für Physik und IRIS-Adlershof, Humboldt-Universität zu Berlin

DFT calculations lead to low-energy effective models. A modern example would be Kitaev types spin Hamiltonains for $RuCl_3$. Once the model is specified, many different many-body calculations can be carried out. Here, we will concentrate on the ALF [1] implementation of the auxiliary field quantum Monte Carlo algorithm that can deal with general models that includes the ones produced by DFT calculations. Being a Monte Carlo method, the ALF library produces stochastic time series. We will discuss how to implement this workflow in the NOMAD Repository & Archive (https://nomad-lab.eu) and concentrate on a FAIR meta-data scheme. The first challenges are to define the models in a searchable way as well as standards for the Monte Carlo time series. In this talk we will discuss the present state of this project for the special case of the ALF-library and how users can exploit the benefits of the NOMAD repository to find, compare and resuse our QMC data.
[1] F. F. Assaad et al., SciPost Phys. Codebases **1** (2022).

O 84.10 Thu 18:00 WIL A317

CAMELS - A Configurable Instrument Control Software for FAIR Data — •Alexander Fuchs[1,3], Johannes Lehmeyer[1,3], Michael Krieger[1,3], Heiko B. Weber[1,3], Patrick Oppermann[2,3], and Heinz Junkes[2,3] — [1]Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft (FHI), Berlin — [3]FAIRmat, Humboldt-Universität zu Berlin, Berlin, Germany

We are developing a configurable measurement software (CAMELS), targeted towards the requirements of experimental solid-state physics. Here many experiments utilize a multitude of measurement devices used in dynamically changing setups. CAMELS [1] will allow to define instrument control and measurement protocols using a graphical user interface (GUI). This provides a low entry threshold enabling the creation of new measurement protocols without programming knowledge or a deeper understanding of device communication. The GUI generates python code that interfaces with instruments and allows users to modify the code for specific applications and implementations of arbitrary devices if necessary. Even large-scale, distributed systems can be implemented. CAMELS is well suited to generate FAIR-compliant output data. Nexus standards, immediate NOMAD integration and hence a FAIRmat compliant data pipeline can be readily implemented.
[1] https://github.com/FAU-LAP/CAMELS

O 84.11 Thu 18:15 WIL A317

OpenSemanticLab: Usecase Device Repository — •Matthias A. Popp and Simon Stier — Fraunhofer ISC, Neunerplatz 2, 97082 Würzburg, Germany

Fully automated experiments provide benefits regarding precision, repeatability, as well as data quality and therefore gain more and more popularity. However, setting them up can be time consuming, especially when computer interface information has to be manually transferred from device manuals to software.

In order to implement FAIR principles precise descriptions of measurement setups and instrumentation are necessary. Currently, this results in extra workload for experimental scientists.

With our framework OpenSemanticLab, we address this shortcoming by providing a central metadata repository for scientific instruments. The ontology-based repository meets both human (GUI) and machine requirements (APIs). A device ontology helps finding and classifying devices. In an associated Python package, abstract device drivers and concrete device metadata can be combined into executable workflows. Overall, this approach not only strengthens the transparency of research according to FAIR principles, but also significantly reduces the implementation effort for complex setups.

O 85: Electronic Structure of Surfaces II

Time: Thursday 15:00–17:45 Location: REC C 213

O 85.1 Thu 15:00 REC C 213

Electronic structure of transition metal oxide surfaces from coincident electron spectroscopy — •Danilo Kühn[1], Swarnshikha Sinha[1,2], Artur Born[1,2], Fredrik O. L. Johansson[3], Ruslan Ovsyannikov[1], Nils Mårtensson[3], and Alexander Föhlisch[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Strasse 24-25, 14476 Potsdam, Germany — [3]Department of Physics and Astronomy, Uppsala University, P.O. Box 256, 751 05, Uppsala, Sweden

Transition metal oxides are a much studied class of materials with a wide range of applications, e.g. solar cells, batteries, magnetic storage devices, sensors or pigments. Varying charge localizations in the s,p and d valence shells and coupling between subsystems invoke complex electronic, magnetic and optical phases as high Tc superconductivity. Here, results from the new COESCA station for coincident electron spectroscopy at the BESSY II synchrotron will be presented [Leitner, T. et al. J. El. Spec. 250, 147075 (2021)]. Combining the high transmission and energy resolution of ARTOF time-of-flight spectrometers with the tailored time structure of BESSY II, Auger- Photoelectron coincidence spectroscopy (APECS) is possible with unprecedented information rate in the soft x-ray regime. Exploiting enhanced chemical selectivity and surface sensitivity, we gain insight into the excitation-decay dynamics and electron correlation effects in Ni, Cu and their oxides [Born, A. et al. Sci Rep 11, 16596 (2021)]

O 85.2 Thu 15:15 REC C 213

Black Phosphorus and the Free-Electron Final-State Assumption in Photoemission Spectroscopy — •Charlotte Sanders[1], Klara Volckaert[2], Deepnarayan Biswas[3], Marco Bianchi[2], Philip Hofmann[2], and Irene Aguilera[4] — [1]Central Laser Facility, STFC Rutherford Appleton Lab, Research Complex @ Harwell, OX11 0QX, UK — [2]Dept. of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus-C, DK — [3]Diamond Light Source, Division of Science, Didcot, OX11 0DE, UK — [4]Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH, Amsterdam, NL

In the photoemission process, the in-plane component (k_x, k_y) of the electron wave vector is conserved; but the k_z component is not, due to breaking of out-of-plane symmetry at the surface. This fact complicates analysis of photoemission spectra from k_z-dispersing states.

Bulk black phosphorus has a k_z-dispersing state that has been the subject of several studies wherein photoemission intensity close to the Fermi level resists interpretation on the basis of simple free-electron-like final-state assumptions. Experimental spectra have been interpreted in terms of surface resonances, or of complexities in the final state that go beyond the free-electron assumption. Here we present experimental and theoretical results concerning the latter interpretation; and, we consider the fundamental meaning of the free-electron-like final-state.

O 85.3 Thu 15:30 REC C 213

Direct observation of antiferromagnetic parity violation in the electronic structure of Mn_2Au — •Yaryna Lytvynenko[1,2], Olena Fedchenko[1], Libor Šmejkal[1,3], Michael Kallmayer[4], Katerina Medjanik[1], Sergey Babenkov[1], Dmitry Vasilyev[1], Mathias Kläui[1], Jure Demsar[1], Gerd Schönhense[1], Martin Jourdan[1], Jairo Sinova[1,3], and Hans-Joachim Elmers[1] — [1]Institute of Physics, JGU Mainz — [2]Institute of Magnetism of the NAS and MES of Ukraine — [3]Institute of Physics Academy of Sciences of the Czech Republic — [4]Surface Concept GmbH

Using time-of-flight momentum microscopy with a sub-μm spatial resolution (sub-μ-ToFMM), allowing for momentum-resolved photoemission on individual antiferromagnetic domains, we observe an asymmetry in the electronic band structure, $E(k) \neq E(-k)$, in Mn_2Au. This broken band structure parity originates from the combined time and parity symmetry, PT, of the antiferromagnetic order of the Mn moments, in connection with spin-orbit coupling [1,2]. The spin-orbit interaction couples the broken parity to the Néel order parameter direction. We demonstrate a novel tool to image the Néel vector direction by combining spatially resolved momentum microscopy with ab-initio calculations that correlate the broken parity with the Néel vector [3].

References

1. L. Smejkal et al., Phys. Rev. Lett. 118, 106402 (2017)
2. H.-J. Elmers et al., ACS Nano 14, 17554-64 (2020)
3. O. Fedchenko et al., J. Phys.: Condens. Matter 34, 425501 (2022)

O 85.4 Thu 15:45 REC C 213

Impact of atomic defects in the electronic states of $FeSe_{1-x}S_x$ superconducting crystals — •Yanina Fasano[1,2], Jazmin Aragon Sanchez[1], Maria Lourdes Amigo[1], Esteban Gayone[1], and Gladys Nieva[1] — [1]Instituto Balseiro and Centro Atomico Bariloche, UnCuyo-CNEA, Argentina — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Germany

The electronic properties of Fe-based superconductors are drastically affected by deformations on their crystal structure introduced by doping and pressure. Here we study single crystals of $FeSe_{1-x}S_x$ and reveal that local crystal deformations such as atomic-scale defects impact the spectral shape of the electronic core level states of the material. By means of scanning tunneling microscopy we image S-doping induced defects as well as diluted dumbbell defects associated with Fe vacancies. We have access to the electronic structure of the samples by means of x-ray photoemission spectroscopy (XPS) and show that the spectral shape of the Se core levels can only be adequately described by considering a principal plus a minor component of the electronic states. We find this result for both pure and S-doped samples, irrespective that in the latter case the material presents extra crystal defects associated to doping with S atoms. We argue that the second component in our XPS spectra is associated with the ubiquitous dumbbell defects in FeSe that are known to entail a significant modification of the electronic clouds of surrounding atoms.

O 85.5 Thu 16:00 REC C 213

Double Photoemission Spectroscopy of C_{60} on $SrTiO_3(001)$ with Laser VUV radiation — •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

Via photoelectron spectroscopy, important insights into the electronic structure of solids were obtained. However, correlation effects can only be addressed indirectly. With double photoemission spectroscopy (DPE), such phenomena can be observed directly by detecting pairs of correlated photoelectrons emitted upon absorption of a single photon [1]. C_{60} is classified as a strongly correlated material with a highly structured valence band spectrum. Moreover, theory predicts the possibility of plasmon-mediated pair emission in C_{60} [2]. In this contribution we present DPE data for C_{60} thin films on $SrTiO_3(001)$, obtained by a laboratory high-order harmonic (HHG) light source, operating at an energy range from 14 to 40 eV and MHz repetition rates [3]. We analyze the 2D energy maps and compare the data to the SPE spectrum. In addition, we discuss plasmon-mediated DPE in fullerenes.

[1] J. Berakdar et al., Phys. Rev. Lett. **81**, 3535 (1998)
[2] Y. Pavlyukh et al., Phys. Rev. B **91**, 155116 (2015)
[3] A. Trützschler et al., Phys. Rev. Lett. **118**, 136401 (2017)

O 85.6 Thu 16:15 REC C 213

Electronic structure at the "interface" of spin-orbit and exchange interaction: Ultrathin ferromagnetic films on W(110) — •Pascal Jona Grenz[1], Peter Krüger[1], Marcel Holtmann[1], Koji Miyamoto[2], Shiv Kumar[2], Taichi Okuda[2], and Markus Donath[1] — [1]WWU, Münster, Germany — [2]HISOR, Hiroshima, Japan

Ultrathin ferromagnetic layers on W(110) provide a suitable platform for investigating spin phenomena originating from the interplay of spin-orbit coupling (SOC) and exchange interaction (XC). First, we focus on the influence of ferromagnetic adlayers on the SOC-induced topologically non-trivial surface state (TSS) hosted by the W(110) surface [1,2]. Our systematic angle-resolved photoemission study of thin Ni, Co, and Fe films and their influence on the TSS will be presented and discussed in view of conflicting literature results [3]. Second, the unoccupied electronic structure of thin Ni films on W(110) is surveyed by spin- and angle-resolved inverse photoemission. By carefully choosing the Ni film's thickness, we tune the relative strength of SOC and XC. In such a way, SOC induces a degeneracy of Ni-related exchange-split states. Based on density functional theory, the strong interplay of SOC and XC is traced back to the hybridization of W and Ni states.

[1] K. Miyamoto *et al.*, *Phys. Rev. Lett.* 108, 066808 (2012)
[2] P.J. Grenz *et al.*, *J. Phys.: Condens. Matter* 33, 285504 (2021)
[3] K. Honma *et al.*, *Phys. Rev. Lett.* 115, 266401 (2015)

O 85.7 Thu 16:30 REC C 213

Circular dichroism in angle-resolved photoemission from core-level emission of W(110) — •Trung Phuc Vo[1], Olena Tkach[2,3], Katerina Medjanik[2], Olena Fedchenko[2], Hans-Joachim Elmers[2], Gerd Schönhense[2], and Ján Minár[1] — [1]New Technologies - Research Centre, University of West Bohemia, 301 00 Pilsen, Czech Republic — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, D-55128 Mainz, Germany — [3]Sumy State University, Rymski-Korsakov 2, 40007 Sumy, Ukraine

Angle-resolved photoemission spectroscopy (ARPES) is a driving experimental technique for examining the electronic structure of quantum materials. There is another technique called X-ray photoelectron diffraction (XPD) which is considered to be the same thing as ARPES from an elementary point of see, specifically the angular distribution of photoelectrons emitted from a crystal surface. Nevertheless, the angular distribution of emitted electrons represents the momentum of initial states in ARPES meanwhile it reveals the interference of photoelectron waves from final states in XPD. At high photon energies, photoelectron diffraction (PED) effects are found in ARPES measurements beside other obstacles (e.g. non-negligible phonon scattering). Here, to disentangle these diffraction influences, we present a PED implement for SPRKKR package which makes use of multiple scattering theory and one-step model in photemission process. For the sake of applications, we have calculated the circular dichroism in angular distributions (CDAD) associated with of 4f and 3d states from W(110). Photoelectrons are excited by hard X-rays (6000 eV).

O 85.8 Thu 16:45 REC C 213

Automatic Quantification of Transitional Metal X-ray Photoelectron Spectra using Convolutional Neural Networks — •Lukas Pielsticker, Walid Hetaba, and Mark Greiner — Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany

In X-ray photoelectron spectroscopy (XPS), quantitative analysis of the nature and composition of surface chemical species is typically performed manually through empirical curve fitting by expert spectroscopists. However, recent advancements in the ease-of-use and reliability of XPS instruments have led to ever more (novice) users creating increasingly large data sets that are becoming harder to analyze by hand. Reflecting this development, more automated analysis techniques are desirable to aid these users with the analysis of big XPS datasets. Here we show that by training convolutional neural networks (CNN) on artificially generated XP spectra with known quantifications (i.e., for each spectrum, the concentration of each chemical species is known), it is possible to obtain models for auto-quantification of transition metal XP spectra. CNNs are shown to be capable of quantitatively determining the presence of metallic and oxide phases, achieving competitive accuracy as more conventional data analysis methods. The proposed networks are flexible enough to accommodate spectra containing multiple chemical elements and measured with different experimental settings. The use of dropout variational inference for the determination of quantification uncertainty is discussed.

O 85.9 Thu 17:00 REC C 213

Revisiting the Strongly Correlated Si-terminated 3C-SiC(100)-p(2×1) Surface with Density- and Wave Function-Based Methods — •Niklas Thoben and Thorsten Klüner — Carl von Ossietzky Universität, Oldenburg, Germany

Silicon carbide is an environmentally friendly, abundant and chemically stable wide band gap semiconductor. From the numerous known polytypes, cubic silicon carbide (3C-SiC) shows the lowest band gap with 2.36 eV, which straddles the water redox potentials and thus making this material a possible candidate for photoelectrochemical water splitting [1]. 3C-SiC is generally obtained as thin films on Si(100) substrates [2], resulting in the 3C-SiC(100) surface being the most common surface. In the Si-terminated case, this surface can exhibit a p(2×1) reconstruction with symmetric Si-dimers [3]. In literature, this system has almost exclusively been described by periodic closed shell density functional theory (DFT) even though the symmetric dimers should be strongly correlated and thus show open shell and multi-configurational character to a certain extent.
Consequentially, in this contribution we apply spin-polarized periodic hybrid DFT and multi-configurational wave function-based methods on the 3C-SiC(100)-p(2×1) surface.

[1] J. Jian, J. Sun, *Sol. RRL* **2020**, *4*, 2000111.
[2] V. Jokubavicius *et al.*, *Cryst. Growth Des.* **2014**, *14*, 6514.
[3] J. Pollmann, J. Krüger, *J. Phys.: Condens. Matter* **2004**, *16*, 1659.

O 85.10 Thu 17:15 REC C 213

Coulomb potential truncation in hybrid calculations — •Kristians Kacars and Andris Gulans — University of Latvia

Solving Poisson's equation is a fundamentally important part of electronic structure calculations. The long-range character of the Coulomb potential makes this task non-trivial in a range of applications. It leads to diverging Fock exchange and spurious interactions of periodic images of low-dimensional systems in supercell calculations. We address this problem in the context of linearized augmented plane waves(LAPW), considering two different approaches to extending Weinert's method. In the first of them, we employ a wavelet-based Poisson equation solver from the *psolver* library. In the second one, we use Coulomb potential truncation schemes. Both approaches are implemented and tested in the LAPW code `exciting`. We apply and compare these methods for bulk materials and low-dimensional systems in calculations with local and hybrid functionals.

O 85.11 Thu 17:30 REC C 213

Ultra-fast machine learning potentials for hydrogen under pressure — •Thomas Bischoff[1], Bastian Jäckl[1], and Matthias Rupp[1,2] — [1]Department of Computer and Information Science, University of Konstanz, Germany — [2]Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), Luxembourg

Hydrogen exhibits remarkably complex behavior at high pressures. Its rich phase space with multiple solid and liquid polymorphs is the subject of controversial scientific debate [1,2].

We apply ultra-fast potentials (UFPs) to model hydrogen under pressure. UFPs are recent robust interpretable machine-learning potentials that enable accurate simulations of large atomistic systems over long time scales [3].

We examine the accuracy of UFPs for training data from density functional theory and quantum Monte Carlo calculations. We also demonstrate the physical interpretability of UFPs for reference configurations composed of atomic and molecular hydrogen. With the obtained machine-learning potential, we investigate solid-liquid and liquid-liquid phase transitions for an extensive part of the phase diagram of dense hydrogen.

[1] (a) B. Cheng et al., *Nature* 585: 217, 2020; (b) V.V. Karasiev et al., *Nature* 600: E12, 2021; (c) B. Cheng et al., *Nature* 600: E15, 2021.
[2] A. Tirelli et al., *Physical Review B* 106(4): L041105, 2022.
[3] S. R. Xie et al., *arXiv 2110.00624*, 2021.

O 86: Solid-Liquid Interfaces II: Reactions and Electrochemistry I

Time: Thursday 15:00–17:45 Location: TRE Phy

O 86.1 Thu 15:00 TRE Phy

Enter the Void: Cavity Formation at Metal-Water Interfaces — •Thorben Eggert[1,2], Nicolas G. Hörmann[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Technical University of Munich, Munich, Germany

Cavity formation is an important concept when rationalizing the solvation of ions. However, most studies only analyze cavities in bulk liquids, omitting that their properties may change dramatically at solid-liquid interfaces.

Here, we study cavities at interfaces, particularly their free energy of formation based on classical molecular dynamics simulations. Specifically, we use a particle insertion approach, as well as thermodynamical integration via the Multistate Bennett Acceptance Ratio. We demonstrate that cavity formation at interfaces depends on the substrate material, which can be rationalized by the strength of the substrate-water interaction. Furthermore, we observe deviations from the bulk behavior in the second solvation layer, which underlines the importance of the substrate-specific interfacial water structure. Finally, we validate our findings with *ab initio* molecular dynamics simulations.

These results allow a quantification of the competitive nature of adsorption processes at solid-liquid interfaces. Ultimately, they could improve implicit solvation models, which typically neglect substrate-specificity.

O 86.2 Thu 15:15 TRE Phy

first-principles molecular dynamics simulations of electrified Pt(111)/H2O interfaces — •Lang Li[1,2], Nicolas Hörmann[1], and Karsten Reuter[1] — [1]Fritz haber institut of Max planck socirty — [2]Humboldt-Universität zu Berlin

Metal-water interfaces play a fundamental role in electrochemistry. An accurate understanding of their properties is required in any attempt to describe electrochemical phenomena such as electrocatalytic reactions or charge transfer processes.

In this work, we benchmark the description of electrified Pt(111)/water interfaces based on first-principles molecular dynamics simulations at applied potential conditions using density functional theory. We apply the potential by introducing excess electrons that are counterbalanced by partially charged hydrogen atoms. This method is tested with a variety of slab setups and cell sizes.

We analyze in detail the structure of the interface as well as the obtained capacitance vs. potential curves and compare these with published theoretical and experimental results [1]. Our results highlight the response of interfacial water to an applied potential and its importance for understanding the hump in the capacitance, observed at high electrolyte concentrations [2].

[1] L. Li, J. -B. Le, J. Cheng, Cell Rep. Phys. Sci., 3, 100759 (2022).
[2] J.B. Le, Q.Y. Fan, J.Q. Li, J. Cheng, Sci. Adv., 6, eabb1219 (2020).

Topical Talk O 86.3 Thu 15:30 TRE Phy

Novel concepts to simulate electrified liquid/solid interfaces from first principles — Florian Deissenbeck[1], Christoph Freysoldt[1], Mira Todorova[1], Jörg Neugebauer[1], and •Stefan Wippermann[1,2] — [1]Max-Planck-Institut für Eisenforschung — [2]Philipps-Universität Marburg

Ab initio techniques have revolutionized the way how theory can help practitioners to discover and design new materials, and explore critical mechanisms. Achieving an atomistic understanding of electrochemical processes is imperative to realize disruptive innovations, e.g. power-to-X devices, supercapacitors, metal-air batteries, new concepts in sustainable metallurgy. A well known example, how novel concepts can impact our ability to perform such studies is the introduction of temperature control into *ab initio* simulations. The analogous technique to model electrochemical systems - potential control - is just emerging.

We recently introduced a “thermopotentiostat”: a novel approach to control the electrode potential in molecular dynamics (MD) simulations [1], that can be straightforwardly implemented into any density-functional code [2]. Here, we provide a perspective on the key concepts of simulating electrified liquid/solid interfaces via *ab initio* MD at controlled electrode potential. To highlight the opportunities provided by these developments we discuss the dielectric response and splitting of liquid water in contact with electrified semiconductor surfaces.

[1] F. Deißenbeck, C. Freysoldt, M. Todorova, J. Neugebauer, S. Wippermann, Phys. Rev. Lett **126**, 136803 (2021)

[2] F. Deißenbeck, S. Wippermann, arXiv:2209.04363

O 86.4 Thu 16:00 TRE Phy

Entropic contributions to the stability of electrochemically adsorbed anion layers on Au(111), a microcalorimetric study — •Marco Schönig and Rolf Schuster — Karlsruhe Institute of Technology, Germany

The understanding of the solid/electrolyte interface is detrimental for rationalizing of electrochemical processes. In this contribution we use electrochemical microcalorimetry to study the entropy of formation of the interface for anion (Cl^-,Br^-,I^-,SO_4^{2-}) adsorption on Au(111) [1]. The entropy of formation of the interface provides information on the structure, order and composition of this interface, which are often used as descriptors in electrochemical processes. The specific adsorption of anions on Au(111) is an important model system, since the nearly ideal polarizability of the gold surface over a large potential window allows to study the formation of surface adlayers up to high surface coverages. We found a negative reaction entropy during the adsorption process, with a distinct minimum around two thirds of the maximum coverage. Additionally, we observed that the course of the reaction entropy vs. potential changes with the employed cation (Li^+,K^+,Cs^+) in solution. We will discuss contributions of the solvent and the electrolyte to the entropy of formation of the interface and provide statistical mechanics models to describe the measured data. We found that it was imperative to include repulsive interactions between the adsorbates to account for the experimental results. [1] M. Schoenig and R. Schuster Phys. Chem. Chem. Phys., 2022, Accepted Manuscript

O 86.5 Thu 16:15 TRE Phy

Impact of confined water on solvation and adsorption/desorption energetics of charged ions at the electrified interface — •Zhenyu Wang, Mira Todorova, and Jörg Neugebauer — Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Str.-1, D-40237, Düsseldorf, Germany

Understanding processes at electrified solid/liquid interfaces is crucial for many systems and a wide range of applications in the electrochemical industry, catalytic sciences and biological engineering. Using a prototypical model system of a single ion in water confined between two charged electrodes, we perform nanosecond-scale atomistic molecular dynamics simulations to study the dielectric behavior of chemically pure water as well as the solvation of ions in the presence of an electric field. For weak electric fields, we find that the screening charge density of water is proportional to the external electric intensity, in agreement with classical polarization theory. Probing the interface structure by the single Na+/Cl- ion we investigate the formation and evolution of the ion’s solvation shell as a function of the electrode-ion distance. Comparing potential profiles from Na+/Cl- calculations for different charge states and positions, we elucidate the role of screening and solvation shell size on reorganization energies and the transmission barrier of the ions close to the interface.

O 86.6 Thu 16:30 TRE Phy

Dynamics of the Iridium-Oxide/Water Interface from Machine Learning Potential Simulations — •Nikhil Bapat, Simon Wengert, Hendrik H. Heenen, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

The interaction of liquid water with a solid substrate at an electrified solid/liquid interface plays a crucial role in the activity and stability for electrocatalysts such as IrO_2. It is therefore important to obtain detailed insights about the underlying processes on these interfaces. Here, resolving the dynamical evolution at the atomic scale requires highly accurate yet efficient models that overcome the length and time scale restrictions imposed by traditional *ab initio* molecular dynamics simulations. To that end, we use the Gaussian approximation potential framework to construct a machine-learned model trained on density-functional theory data for the IrO_2(110)/water interface. The established training protocol uses an automated and iterative procedure to ensure that the training data covers the *a priori* unknown geometric and compositional motifs of the evolving working interface.

The model is then used to run reactive molecular dynamics simulations with varying surface compositions. Crucial for electrolysis, the reduced computational cost allows to efficiently explore the diverse configuration space of adsorbed intermediates in the oxygen evolution reaction. Furthermore, we investigate the mobility of water in dependence of the underlying surface composition in which, long-range effects are reflected in a strong variation of water mobility as a function of distance to the surface.

O 86.7 Thu 16:45 TRE Phy

First-principles study of electrochemical effects in Si/SiOx-water interfaces — •Kamila Savvidi[1] and Robert H. Meissner[1,2] — [1]Institute of Polymer and Composites, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Surface Science, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Nanoporous silicon is a prominent candidate for application in energy storage devices as silicon can be conductive under certain conditions. Computer simulations offer an understanding of the electrified semiconductor/water interfaces on the atomistic level; essential for the efficient design and optimization of these devices. We use *ab-initio* molecular dynamics (AIMD) to study the capacitive properties of Si/water interface in the presence of an electrostatic potential. A doped Ne crystal is used as counter electrode to a SiO_x slab and to a hydrogenated Si(100) slab to apply a constant bias potential while explicit water molecules constitute the electrolyte solution.[1] Differential capacitance is estimated by the time-averaged atomic charge fluctuations for each system. To obtain more information about the influence of individual electrode atoms to the differential capacitance, the charge fluctuations of each atom are used to calculate a charge-charge covariance matrix $\mathbf{K}^{-}_{\mathrm{qq}}$. [2] Results are compared to the simulation of a single electrode with water on either side in an electric field.

[1] S. Surendralal *et al.*, Phys. Rev. Lett. 120, 246801 (2018)

[2] J. Seebeck, C. Merlet, R. H. Meißner, Phys. Rev. Lett. 128, 086001 (2022)

O 86.8 Thu 17:00 TRE Phy

Thermodynamic Cyclic Voltammograms from First Principles — •Nicolas Bergmann, Nicolas G. Hörmann, and Karsten Reuter — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Cyclic voltammograms (CVs) are a central experimental tool for assessing the structure and activity of electrochemical interfaces. Computationally, a predictive-quality modeling of CVs is challenging due to the entangled need to accurately account for the interactions and reactive chemistry at the liquid electrolyte/solid electrode interface as well as for the applied potential [1]. For sufficiently small scan rates, thermodynamic approaches help to meet these challenges.

Here, we compare different options to derive thermodynamic CVs consistently and at low computational cost, using the well-studied model system of Ag(100) in a Br-containing electrolyte as a test case. We present our generalized ansatz to derive continuous expressions within a mean-field (MF) model, using non-parametric Gaussian process regression. We also shine light on the inherent accuracy limitations of MF theory, by comparing it to CVs from grand-canonical lattice Monte Carlo simulations. Finally, we show how augmenting traditional zero-field calculations (computational hydrogen electrode, CHE) with capacitive double layer energetics (CHE+DL) [1] within an implicit solvent model influences the theoretical results.

[1] N.G. Hörmann et al., J. Chem. Theory Comput. 2021, 17, 1782

O 86.9 Thu 17:15 TRE Phy

Electrodeposition and Electrochemical Characterization of Thin Nickel Overlayers on Au(111) — •Markus Wittmann, Ludwig A. Kibler, and Timo Jacob — Ulm University, Institute of Electrochemistry, 89069 Ulm, Germany

Nickel is widely used in energy storage and conversion, *e.g.* nickel–iron, nickel–cadmium, and nickel–metal hydride batteries. The behavior of nickel electrodes has been investigated extensively. However, a detailed understanding of adsorption and absorption processes on the atomic level is still missing. In particular, the distinction between surface and bulk atoms, as well as adsorbed hydrogen during electrooxidation is difficult.[1,2] Here we report on the electrochemical fabrication of thin nickel overlayers on Au(111) and their electrochemical characterization. Stable nickel overlayers have been electrochemically deposited onto Au(111) from a 1 mM $NiSO_4$ solution and subsequently characterized by cyclic voltammetry in a 10 mM KOH solution. The current density–potential curves of nickel overlayers on an Au(111) single crystal in comparison with the behavior of Au(111) and Ni(111) in 10 mM KOH help separating surface and bulk contributions of nickel electrooxidation. This is especially relevant for small deposits with a high surface-to-bulk ratio. In addition, relations between the structure of the nickel electrodeposit and its electrochemical behavior are addressed.

[1] D. S. Hall et al., J. Electrochem. Soc. **160** (2003) 235–243.
[2] L. F. Huang et al., J. Phys. Chem. C **121** (2017) 782–9789.

O 86.10 Thu 17:30 TRE Phy

Cu Underpotential Deposition on Au(111) in Presence of Carboxylic Acids — •Sebastian Fackler, Markus Wittmann, Ludwig A. Kibler, and Timo Jacob — Ulm University, Institute of Electrochemistry, 89069 Ulm, Germany

The underpotential deposition (UPD) of foreign metals on different host metals has been extensively studied, especially for Cu on Au(111).[1] Apart from the nature of the metals, the nature and concentration of anions in the solution govern the initial stages of the deposition process. The influence is usually explained with respect to non-specific and specific adsorbing anions, with the ability of the latter to stabilize sub-monolayers of the deposited metal on the host metal by co-adsorption on top of well-ordered superstructures.[1]

Similarities and differences of the Cu UPD on Au(111) with short-chained carboxylic acids in comparison with known inorganic anions were systematically investigated by cyclic voltammetry and current transients. Despite the non-specifically adsorbing nature of perchlorate ions, the present study demonstrates that perchlorate can influence the Cu deposition in presence of specifically adsorbing acetate ions. Similarly, it has been found by in-situ STM studies that the presence of perchlorate influences the adsorption structure of strongly adsorbing formate on Au(111).[2]

[1] E. Herrero, et al., Chem. Rev. 2001, 101, 187-1930.
[2] A. Abdelrahman, Dissertation, Ulm University, 2019.

O 87: Focus Session: Scanning Probe Microscopy with Quartz Sensors III

Time: Thursday 15:00–17:30 Location: TRE Ma

Topical Talk O 87.1 Thu 15:00 TRE Ma

Quartz-sensor detection for single-electron tunneling spectroscopy — •Jascha Repp — Department of Physics, University of Regensburg, 93040 Regensburg, Germany

We exploit the high sensitivity of qPlus-based [1] atomic force microscopy (AFM) to perform scanning tunneling microscopy (STM) and spectroscopy on molecules in absence of any conductance of the underlying substrate. Thereby, we gain access to out-of-equilibrium charge states that are out of reach for conventional STM [2]. Extending this technique by electronic pump-probe spectroscopy [3], we measured the triplet lifetime of an individual pentacene molecule on an insulating surface [4] and lifetime quenching by nearby oxygen molecules. Combined with radio-frequency magnetic-field driving we introduce AFM-based electron spin resonance and spin manipulation showing long spin coherence in single molecules.

References: [1] F. J. Giessibl, Appl. Phys. Lett. 73, 3956 (1998). [2] L. L. Patera et al., Nature 566, 245 (2019). [3] S. Loth et al., Science 329, 1628 (2010). [4] J. Peng et al., Science 373, 452 (2021).

O 87.2 Thu 15:30 TRE Ma

molecular diffusion studied by multidimensional cantilever-based UHV AFM — •Zuned Ahmed[1,2], Hao Liu[1,2], Manfred Parschau[1], and Hans Josef Hug[1,2] — [1]Empa (Swiss Federal Laboratories for Materials Science and Technology), Dübendorf , Switzerland — [2]University of Basel, Switzerland

Scanning probe microscopy permits a characterization of the diffusion of atoms or molecules on surfaces, which is governed by diffusion energy barrier and entropy difference between ground and excited states. With our home-built, cantilever based UHV, low temperature scanning force microscope [1], we studied the diffusion of benzene-based molecules with flexible and rigid hydrocarbon chains, namely,1,3,5-Triethylbenzene (TEB) and 1,3,5-Trimethylbenzene (TMB), respectively, measured at temperatures between 6.38 and 10.68 K on Cu (111). An Arrhenius analysis revealed that the molecule with the flexible hydrocarbon arms (TEB) showed an enhanced diffusion rate which we can attribute to its higher configurational entropy of its ethyl chains. Moreover, we used multidimensional AFM to map the vertical and lateral forces required to manipulate both molecules. Compatible with the lower diffusion energy barrier of the TEB molecule, the force required to manipulate the TEB was much smaller than that of the TMB molecule. In addition, the measured flexural and torsional frequency shift data permitted a detailed analysis of the manipulation process.

[1] Liu et al. Beilstein J. Nanotechnol. 2022, 13, 1120-1140

O 87.3 Thu 15:45 TRE Ma

Flexible Superlubricity Unveiled in Snake-Like motion of Individual Chains — •Guilherme Vilhena[1,2], Rémy Pawlak[1], Philipp D'Astolfo[1], Xunshan Liu[3], Enrico Gnecco[4], Marcin Kisiel[1], Thilo Glatzel[1], Rúben Pérez[2], Robert Häner[3], Silvio Decurtins[3], Alexis Baratoff[1], Giacomo Prampolini[5], Shi-Xia Liu[3], and Ernst Meyer[1] — [1]University of Basel, Switzerland — [2]Universidad Autónoma de Madrid, Spain — [3]University of Bern, Switzerland — [4]Jagiellonian University, Poland — [5]Consiglio Nazionale delle Ricerche, Italy

A combination of low-temperature atomic force microcopy and molecular dynamic simulations demonstrates that soft designer molecules realize a sidewinding motion when dragged over a gold surface. Exploiting their longitudinal flexibility, pyrenylene chains are indeed able to lower diffusion energy barriers via on-surface directional locking and molecular strain. The resulting ultralow friction reaches values on the order of tens of pN reported so far only for rigid chains sliding on an incommensurate surface. Therefore, we demonstrate how molecular flexibility can be harnessed to realize complex nanomotion while retaining a superlubric character. This is in contrast with the paradigm guiding the design of most superlubric nanocontacts (mismatched rigid contacting surfaces).

O 87.4 Thu 16:00 TRE Ma

Machine learning for high-resolution AFM image interpretation — •Niko Oinonen[1], Lauri Kurki[1], Chen Xu[1], Shuning Cai[1], Markus Aapro[1], Alexander Ilin[2], Peter Liljeroth[1], and Adam Foster[1,3] — [1]Department of Applied Physics, Aalto University, Finland — [2]Department of Computer Science, Aalto University, Finland — [3]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Japan

State-of-the-art non-contact atomic force microscopy (AFM) setups operating in vacuum at low temperatures are able to resolve features on the scale of individual atoms in molecules [1]. However, the process of interpreting the resulting AFM images is often a very challenging task even for highly trained experts in the field. We are working towards greater interpretability and greater automation of the processing of AFM images using machine learning methods. We have introduced an approach based on convolutional neural networks for discovering the atomic structure and electrostatic properties of samples directly from AFM images via image descriptors that characterize the sample [2]. Our recent work refines the geometry prediction task by predicting the molecule graph of the sample using a model based on graph neural networks [3]. The current challenge is in generalizing from simulated training data to experimental test data, where we find that the choice of the training data becomes very important.

[1] L. Gross et al., Science, vol. 325, no. 5944, pp. 1110–1114, 2009.
[2] N. Oinonen et al., ACS Nano, 16, 1, 89–97, 2022.
[3] N. Oinonen et al., MRS Bulletin 47, 895–905, 2022.

Topical Talk O 87.5 Thu 16:15 TRE Ma

Application of atomic force microscopy with quartz sensors to

quantum states in graphene and related twisted heterostructures — •Joseph Stroscio — National Institute of Standards and Technology, Gaithersburg, MD, USA.

Atomic force microscopy (AFM) with quartz sensors pioneered by Franz Giessibl has opened many applications in quantum nanoscience where AFM measurements can be made simultaneously and conveniently with scanning tunneling microscopy measurements (STM). In this presentation I will review our work using combined AFM/STM measurements to give a microscopic view of the quantum states in single layer graphene and in twisted graphene heterostructures. In single layer graphene, electrostatic pn junction boundaries provide a convenient geometry for the examination of quantum Hall edge states with microscopic probes. For a graphene Hall bar device defined and tunable by dual gates, we carry out simultaneous AFM, STM, and electrical transport measurements in the system which we developed for detailed measurements of two-dimensional devices in-operando at mK temperatures and in magnetic fields up to 15 T. The AFM, operated in the Kelvin probe force microscopy (KPFM) mode, detects the chemical potential transitions when Landau levels are being filled or emptied as a function of back gate potential with the same fidelity as the scanning tunneling spectroscopy measurements. With KPFM we can map the dispersion of the Landau levels across the quantum Hall edge boundary as a function of density and spatial position.

O 87.6 Thu 16:45 TRE Ma

On the origin and elimination of cross coupling between excitation and tunneling current in scanning probe experiments that utilize the qPlus sensor — •Michael Schelchshorn — Institute of Experimental and Applied Physics, University of Regensburg, Universitätsstraße 31, 93053 Regensburg

The qPlus sensor is a stiff quartz cantilever that facilitates high-resolution combined STM/AFM [1]. Both a tunneling current and the deflection signal resulting from the forces at the tip are measured simultaneously; however, unwanted cross coupling between the tunneling current signal and the excitation of the sensor oscillation can occur. At one bias polarity, this cross coupling acts as an excitation of the oscillation, in the opposite bias it appears as a damping.

This unwanted effect has been observed since the early years of combined STM/AFM experiments using qPlus sensors, but was difficult to explain. Here, we present a new theory that explains this phenomenon, supported by experiments and supplemented by verified measures on how to prevent or at least minimize cross talk. [2]

[1] F.J. Giessibl, The qPlus sensor: a powerful core for the atomic force microscope, Rev. Sci. Instrum. 90, 011101 (2019).

[2] M. Schelchshorn, On the origin of cross coupling between excitation and tunneling current in combined STM/AFM qPlus experiments, University of Regensburg, B.Sc. thesis (2022)

O 87.7 Thu 17:00 TRE Ma

Fe adsorbates and their effect on the surfaces of topological insulators TlBiSe$_2$ and Bi$_2$Se$_3$ — •Adrian Weindl, Christoph Setescak, Emma Grasser, Alexander Liebig, and Franz J. Giessibl — University of Regensburg, Regensburg, Germany

Can one tailor the properties of the topological surface state (TSS) of topological insulators (TIs) by magnetic doping of the TI material? Here, we study the effect of magnetic adatoms on TI surfaces by combined scanning tunneling microscopy (STM) and atomic force microscopy (AFM). Two archetypical TIs, Bi$_2$Se$_3$ and TlBiSe$_2$, are analyzed, which both have relatively large band gaps with their Dirac points well isolated and far from bulk states. Magnetic impurities, in this case single Fe adatoms, and their influence on the local density of states (LDOS) of the two TIs are investigated by scanning tunneling spectroscopy. We detect resonances in the LDOS for both surfaces that arise due to the scattering of electrons in the TSS at these impurities. The position and shape of these resonances are a function of the exact adsorption position of the adatoms, which can be determined by atomically-resolved AFM measurements. In addition, we detect a relaxation of surface atoms due to the presence of Fe adatoms on Bi$_2$Se$_3$. The charge state of the Fe adatoms is determined by Kelvin probe force spectroscopy.

O 87.8 Thu 17:15 TRE Ma

The (2x1) reconstruction of calcite(104) — Jonas Heggemann[1], Yashasvi Ranawat[2], Ondřej Krejčí[2], Adam S. Foster[2], and •Philipp Rahe[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany — [2]Department of Applied Physics, Aalto University, Helsinki FI-00076, Finland

Calcite is an abundant material in the Earth's crust, a central constituent of biominerals in living organisms [1], and currently investigated as a capture material for CO2 [2]. Despite intensive studies, however, there is still serious ambiguity regarding the properties of this surface due to conflictive conclusions for the so-called row-pairing [3] and (2x1) reconstruction [4].

Here, we use a combination of non-contact atomic force microcopy (NC-AFM) with CO-functionalized tips at 5K, density functional theory with state-of-the-art dispersion corrections, and NC-AFM image simulations to clarify the microscopic geometry of calcite(104). A (2x1) reconstruction and a glide plane symmetry is consistently found in the NC-AFM data and DFT results. Most importantly, we identify two different adsorption positions for CO molecules within the (2x1) unit cell. These findings are most critical for future studies where processes on calcite(104)-(2x1) are influenced by the surface geometry.

[1] L. Addadi, S. Weiner, Angew. Chem. Int. Ed. Engl. 31, 153 (1992). [2] P. A. E. Pogge von Strandmann, et al., Nat. Commun. 10, 1983 (2019). [3] A. L. Rachlin, et al., Am. Mineral. 77, 904 (1992). [4] S. L. S. Stipp, et al., Geochim. Cosmochim. Acta 58, 3023 (1994).

O 88: Members' Assembly

Topics: Report of the Chairman, Presentation of the Gerhard Ertl Young Investigator Award, Miscellaneous

Time: Thursday 19:00–19:30 Location: HSZ 01

All members of the Surface Science Division are invited to participate.

O 89: Post-Deadline Session

Time: Thursday 19:30–20:30 Location: HSZ 01

Contributed Post-Deadline Talks

O 90: Overview Talk Karl-Heinz Ernst

Time: Friday 9:30–10:15 Location: TRE Phy

Invited Talk O 90.1 Fri 9:30 TRE Phy

Molecular Surfaces With a Twist: Magnetochiral Asymmetries and Topological Self-Assembly — •Karl-Heinz Ernst — Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf (Switzerland) — Nanosurf Laboratory, Institute of Physics, The Czech Academy of Sciences, Prague (Czech Republic) — Department of Chemistry University of Zurich, Zurich (Switzerland)

Surfaces functionalized with helically shaped aromatic hydrocarbons, so-called helicenes, are of interest for chiroptical electronic devices or for electron spin filtering. After a general introduction into the topic we will report a unique transmission of chirality from single polyaromatic hydrocarbons into two-dimensional self-assembled monolayers on a silver surface. A helicene with relatively high molecular flexibility allows adaptation of handedness during crystal growth which is governed rather by entropy than by enthalpy. The layer is dominated by motifs, such as nodes of different topology, i.e., two-armed and three-armed spirals, and by enantiospecific lateral offset of oligomeric triangles. To our knowledge such chiral self-assembly phenomenon has been neither reported previously nor has such aperiodic tiling of the plane been previously described by geometers. Moreover, we will report spin-selective electron transport phenomena and enantioselective magnetochiral interactions of helicenes with ferromagnetic surfaces by means of photoelectron spectroscopy, spin-polarized low-energy electron microscopy and spin-polarized scanning tunneling microscopy.

O 91: Plasmonics and Nanooptics V: Waveguides and Antennas

Time: Friday 10:30–12:45 Location: CHE 89

O 91.1 Fri 10:30 CHE 89

Intermediate-field coupling of single epitaxial quantum dots to plasmonic nanowires — •Michael Seidel[1], Yuhui Yang[2], Saimon Covre Da Silva[3], Thorsten Schumacher[1], Armando Rastelli[3], Stephan Reitzenstein[2], and Markus Lippitz[1] — [1]Experimental Physics III, University of Bayreuth, Germany — [2]Institute of Solid State Physics, TU Berlin, Germany — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Austria

Integrated plasmonic nanocircuits are highly promising building blocks for future quantum optical applications. In combination with self-assembled epitaxially grown GaAs quantum dots as stable, bright and narrow-band single-photon sources, ultra-compact nanocircuits operating below the diffraction limit can be designed [1]. A crucial aspect is the coupling of the quantum dot emission into plasmonic waveguide modes. Typically, quantum emitters are placed in the optical near-field of a waveguide, imposing high demands on controlled nanofabrication. Furthermore, plasmonic waveguiding is drastically attenuated near high-index dielectrics due to radiative losses. We overcome these challenges by introducing a 100nm thick dieletric spacer layer, which effectively increases the propagation length and preserves acceptable coupling efficiency, resulting in a robust coupling scheme which is difficult to achieve in the near-field. We characterize the nanostructure by low-temperature photoluminescence and cathodoluminescence imaging and find good agreement to numerical simulations.

[1] Wu et al., Nano Lett. 2017, 17, 7, 4291-4296

O 91.2 Fri 10:45 CHE 89

How to obtain modes in optical fibers — •Sergei Gladyshev, Adria Canos Valero, and Thomas Weiss — Institute of Physics, University of Graz, Universitätsplatz 5, 8010 Graz, Austria

Nowadays, new and complex types of optical fibers such as bandgap photonic crystal fibers and antiresonant fibers are actively studied. To understand the physical mechanisms in such fibers, numerical modeling is of great importance. However, numerical calculations for these fibers are extremely challenging. We present an efficient numerical method for obtaining fiber modes in these systems. More specifically, we adapt the contour integral method, a method for solving nonlinear eigenvalues problems, to derive the propagation constant and the electromagnetic near fields of several modes simultaneously.

O 91.3 Fri 11:00 CHE 89

Directional transport in plasmonic waveguide arrays in the presence of disorder — •Anna Sidorenko and Stefan Linden — Physikalisches Institut, Friedrich-Wilhelms-Universität Bonn, Kreuzbergweg 24, 53115-Bonn, Germany

Evanescently coupled waveguides provide a convenient platform for the simulation of various quantum phenomena whose experimental realization in analogous condensed matter systems is otherwise difficult. The basis for this is the mathematical equivalence of the coupled mode theory equations and the discrete Schrödinger equation in the tight-binding approximation. Here we present a comparative study of the robustness of directional transport in presence of disorder in two periodically driven waveguides systems - ratchets [1] and fast Thouless pumps [2]. Directional transport in a ratchet requires fine-tuning of the driving parameters. In contrast, directional transport in Thouless pumping is a topological effect that exists for a range of driving frequencies considering the closed cycle in parameter space. We analyze the effect of topological protection on directional transport by introducing identical disorder distributions to both systems.

References:

[1] Z. Fedorova, C. Dauer, A. Sidorenko, S. Eggert, J. Kroha, S. Linden, ”Dissipation engineered directional filter for quantum ratchets”. Physical Review Research 3(1), 013260 (2021).

[2] Z. Fedorova, H. Qiu, S. Linden, J. Kroha, ”Observation of topological transport quantization by dissipation in fast Thouless pumps,” Nature communications 11, 3758 (2020).

O 91.4 Fri 11:15 CHE 89

Spatially resolved nonlinear plasmonics — •Johannes Schust, Florian Mangold, Niklas Metz, Mario Hentschel, Bettina Frank, and Harald Giessen — 4th Physics Institute, Research Center SCoPE, and IQST, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Nonlinear optical plasmonics investigates plasmonic nanoantenna fields with the help of nonlinear spectroscopy. Here we introduce nonlinear spatially resolved spectroscopy (NSRS) which is capable of imaging the k-space as well as spatially resolved single antennas while it is still possible to carry out spectroscopy.

These additional abilities give us the possibility to spatially resolve the THG signal of gold nanoantenna arrays and investigate the homogeneity of the antenna field. Furthermore, we are able to spatially resolve the THG emission centers of the third-order mode and observe their response to tuning the wavelength over the resonance.

In addition, we discovered that by increasing the laser intensity, certain antennas in our array became exceptionally bright. By correlating our spatially resolved nonlinear image with structural SEM data, we can prove that these bright antennas have deformed into a peanut shape. Thus our NSRS setup enables the investigation of the nonlinear self-enhancement process of nanoantennas under intense laser heating.

O 91.5 Fri 11:30 CHE 89

Spatio-spectral metrics in electron energy loss spectroscopy as a tool to resolve nearly degenerate plasmon modes — Michal Horák, Andrea Konečná, Tomáš Šikola, and •Vlastimil Křápek — Brno University of Technology, Czechia

Electron energy loss spectroscopy (EELS) is utilized to characterize localized surface plasmon modes supported by plasmonic antennas (PAs) with excellent spatial resolution, including studies of hybridized modes in dimer PAs [1,2,3]. However, the spectral resolution of EELS is often insufficient to resolve the hybridized modes for weakly coupled dimers.

Here we address this issue for a case study of the dimer PA composed of two gold discs. We analyze four nearly degenerate hybridized dipole modes. With a traditional approach, the modes cannot be experimentally identified with EELS. Therefore, we propose several metrics that employ the spatial and spectral sensitivity of EELS simultaneously. We apply the metrics to experimental EELS data, demonstrating their ability to resolve three of the above-mentioned modes (with transverse bonding and antibonding modes still unresolved), identify them unequivocally, and determine their energies. In this respect, the spatio-spectral metrics increase the information extracted from EELS applied to PAs.

[1] V. Křápek *et al.*, Nanophotonics **9**, 623 (2020).
[2] O. Bitton *et al.*, Nat. Commun. **11**, 487 (2020).
[3] J.-H. Song *et al.*, Nat. Commun. **12**, 48 (2021).

O 91.6 Fri 11:45 CHE 89

From Static to Dynamic Modulation of Second Harmonic Generation from Plasmonic Hotspots — •Jessica Meier[1], Luka Zurak[1], Andrea Locatelli[2], Thorsten Feichtner[1], René Kullock[1], and Bert Hecht[1] — [1]Nano-Optics and Biophotonics Group, Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Department of Information Engineering, University of Brescia, Italy

Plasmonic dimer antennas feature strong intensity enhancement squeezed into nanoscale gaps, which makes them highly attractive for boosting nonlinear processes, such as multiphoton excitation and harmonic generation [1]. Such phenomena, alongside large field enhancement, often require control over the field symmetry in the gap, which is challenging considering the nanometer length scales. Here, by means of strongly enhanced second harmonic (SH) generation, we demonstrate unprecedented control over the field distribution by systematically introducing geometrical asymmetry. We use focused helium ion beam milling of mono-crystalline gold to realize asymmetric-gap dimer antennas in which an ultra sharp tip with 3 nm apex faces a flat counterpart [2]. By tuning the tip opening angle, we systematically vary the field asymmetry, which in turn modulates the release of SH radiation to the far-field. We further extend the concept of inducing local field asymmetry to reversible tuning of the SH signal from a single antenna by applying an external voltage.

[1] P. Dombi et al., Reviews of Modern Physics 92, 025003 (2020).
[2] J. Meier et al., arXiv:2210.14105 (2022).

O 91.7 Fri 12:00 CHE 89

Laser Printing of Plasmonic Dimers on Optical Fiber Tips for Fiber-based SERS — •Paul Vosshage, Francis Schuknecht, and Theobald Lohmüller — Chair for Photonics and Optoelectronics, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität, Königinstraße 10, 80539 Munich, Germany

Raman Spectroscopy through optical fibers offers great flexibility for conducting measurements both in situ and in vivo, but shows limitations due to the weak Raman scattering cross-sections of most molecules and a considerable background introduced by the fiber material itself. However, a strong signal amplification can be obtained via surface enhanced Raman scattering (SERS) by introducing plasmonic hot-spots on the optical fiber tip.

Here, we demonstrate a single-step approach to pattern plasmonic dimer antennas directly onto glass fibers by optical means. A focused laser beam is used to transform a gold nanorod into two nanospheres of equal size via heating. Simultaneously, optical forces are harnessed to print the two spheres onto the fiber tip as a strongly coupled dimer. The resulting plasmonic dimers feature nm-sized gaps, which provide a strong electromagnetic field enhancement required for fiber-based SERS.

O 91.8 Fri 12:15 CHE 89

Reconfiguring magnetic resonances with plasmonic and dielectric phase-change materials — Lukas Conrads, Andreas Hessler, Sebastian Meyer, Konstantin Wirth, Matthias Wuttig, Dimitry Chigrin, and •Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

For miniaturized active nanophotonic components, resonance tuning of nanoantennas is a key ingredient. Phase-change materials (PCMs) have been established as prime candidates for non-volatile resonance tuning based on a change in refractive index [1]. Currently, a novel material class of switchable infrared plasmonic PCMs, like In_3SbTe_2 (IST), is emerging. Since IST can be locally optically switched between dielectric (amorphous phase) and metallic (crystalline phase) states in the whole infrared range, it becomes possible to directly change the geometry and size of nanoantennas to tune their infrared resonances [2]. Here, crystalline IST split-ring resonators (SRRs) are directly optically written and reconfigured in their arm size to continuously tune their magnetic dipole resonances over a range of 2.4 μm without changing their electric dipole resonances. Furthermore, electric and magnetic dipole resonances of aluminum SRRs covered by the conventional PCM $Ge_3Sb_2Te_6$ can be individually tuned by addressing the hotspots locally [3]. Our concepts are well-suited for rapid prototyping, speeding up workflows for engineering ultrathin, tunable, plasmonic devices for infrared nanophotonics, telecommunications or (bio)sensing.

[1] Wuttig et al., *Nat. Photon.* **11**, 465 (2017) [2] Heßler et al., *Nat. Commun.* **12**, 924 (2021) [3] Conrads et al. *Adv. Mat.* submitted

O 91.9 Fri 12:30 CHE 89

Nanoantenna Electro-Optical-Transducer Utilizing Monolayer WSe_2 — •Patrick Pertsch, René Kullock, Monika Emmerling, Romana Ganser, and Bert Hecht — NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Using light for the communication on computer chips could decrease the power consumption and increase the data bandwidth [1]. To this end, transition-metal-dichalcogenides (TMD), and especially monolayers thereof, are a very promising material class, because they can be used in electronic computing [2] as well as in optical applications [3]. To achieve high integration densities of logical elements, the transducers between electronic and optical signals should be of the same size as the nanoscale transistors used in modern electronics. But so far the photodetectors and emitters based on TMDs are usually much larger.

By combining TMDs with plasmonic nanostructures, the size of the optical elements can be decreased due to the large absorption cross section afforded by the plasmonic nanoantennas. In this work, we demonstrate single plasmonic nanoantennas on monolayer WSe_2 acting as optically-active material. This combination allows to emit and detect light by using only one single nanoscale device.

[1] C. Sun, et. al., Nature 528, 534-538 (2015).
[2] C. Liu, et. al., Nat. Nanotechnol. 15, 545-557 (2020).
[3] Q. Wang, et. al., Nat. Nanotechnol. 7, 699-712 (2012).

O 92: Oxide and Insulator Surfaces II: Structure, Epitaxy and Growth

Time: Friday 10:30–13:00 Location: CHE 91

O 92.1 Fri 10:30 CHE 91

Growth of ultrathin silica films on Pt(111) and Rh(111): Influence of intermixing with the support — •Florian Kraushofer[1], Matthias Krinninger[1], Nils Refvik[2], Friedrich Esch[1], and Barbara Lechner[1] — [1]TU Munich, Germany — [2]University of Alberta, Canada

Silica is a widely used catalyst support material for clusters and nanoparticles. Understanding the relationship between these clusters and the support is challenging, however, because SiO_2 is insulating, and in most applications not crystalline, which limits the use of diffraction-based experimental techniques. Several previous studies have investigated ultrathin, quasi-2D silica films on a variety of metal supports [1], which can then be measured by scanning tunneling microscopy (STM). Previous work on Pt(111) did not result in closed films, which was attributed to lattice mismatch [2]. We show that closed films can in fact be grown on Pt(111) when silica is deposited in excess, likely due to formation of a platinum silicide layer with a slightly expanded lattice constant at the interface. We also report results of film growth on Rh(111), which is a near-perfect match to the lattice constant of freestanding SiO_2 films as calculated by theory. However, no high-quality films were achieved, which we attribute to a different balance of the formation energies for silicide and oxide.

[1] C. Büchner, M. Heyde, Two-dimensional silica opens new perspectives, Prog. Surf. Sci., 92 (2017) 341-374.

[2] X. Yu, B. Yang, J. A. Boscoboinik, S. Shaikhutdinov, and H.-J. Freund, Appl. Phys. Lett. 100 (2012), 151608.

O 92.2 Fri 10:45 CHE 91

Growth of single-phase honeycomb Ti_2O_3 on Pd(111) — •Rajesh Chirala, Stefan Förster, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Transition metal oxides are known to form honeycomb (HC) structures when grown on metal substrates. The oxide-substrate interaction strength defines the substrate-dependent HC lattice parameter. On Au(111), the Ti_2O_3 HC forms a (2×2) superstructure corresponding to lattice parameter of 5.77 Å [1]. On the contrary, Pt(111) has HC relaxing to a lattice parameter of 5.95 Å [2].

Here we study the growth of a Ti_2O_3 HC structure on Pd(111) from the initial stages up to monolayer coverages. The HC is grown by consecutive steps of room-temperature Ti deposition and annealing at 875 K in 7×10^{-9} mbar of O_2. Whilst the smallest HC patches grow with a lattice parameter of 5.8 Å with a rotation of 26° against the $< 1\bar{1}2 >$ direction of Pd(111), they relax to a lattice parameter of 5.95 Å at higher coverage. Due to this relaxation, the HC lattice coincides with the Pd(111) at a rotation of 30°. The implications of this HC structure as template for the growth of dodecagonal oxide quasicrystal will be discussed [3].

[1] F. Sedona et al., J. Phys. Chem. B **109**, 24411 (2005)
[2] C. Wu et al., J. Phys. Chem. C **115**, 8643 (2011)
[3] S. Schenk et al., Nat. Commun, accepted (2022)

O 92.3 Fri 11:00 CHE 91

Magnetite homoepitaxy observed by X-ray intensity growth oscillations — •Steffen Tober[1,2,3], Marcus Creutzburg[1], Björn Arndt[1], Simon Chung[1], Leon Jacobse[1], Arno Jeromin[1], Vedran Vonk[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Centre for X-ray and Nanoscience, Hamburg — [2]Universität Hamburg, Fachbereich Physik — [3]Jülich Centre for Neutron Science (JCNS) and Peter Grünberg Institut (PGI), JARA-FIT, Forschungszentrum Jülich

Processes on the magnetite ($Fe_{3-\delta}O_4$) (001) surface like oxidative regrowth, (partial) lifting of the subsurface cation vacancy reconstruction and the element-specific incorporation of adatoms demonstrate the sensitive relation of oxygen pressure, cation transport and structure in the near-surface region of $Fe_{3-\delta}O_4$ influencing the performance of catalysts and devices [1,2,3]. We exemplarily studied the homoepitaxial growth of $Fe_{3-\delta}O_4$ (001) surface in dependence of the O_2 pressure and iron flux. X-ray intensity growth oscillations proved ordered growth of $Fe_{3-\delta}O_4$ for all probed conditions while atomic force microscopy revealed newly formed micrometre-sized surface structures exceeding the amount of deposited material [4]. Our results indicate the presence of multiple parallel processes during reactive $Fe_{3-\delta}O_4$ homoepitaxy suggesting similar processes to occur also in other applications of $Fe_{3-\delta}O_4$.

[1] Nie et al., J. Am. Chem. Soc. 135, 10091 (2013), [2] Arndt, B. et al. PCCP 22, 8336 (2020), [3] Mirabella et al., Electrochimica Acta, 389, 138638 (2021), [4] van der Vegt et al., Phys. Rev. Lett. 68, 3335 (1992)

O 92.4 Fri 11:15 CHE 91

The dependence of structure on thickness of NiO(100) films on Ag(100) studied by IV-LEED — •Jan Lachnitt[1], Shuvankar Das[2], Krishnakumar S. R. Menon[2], Suman Mandal[3], and Jan I. Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Cottbus, Germany — [2]Surface Physics & Material Science Division, Saha Institute of Nuclear Physics, Kolkata, India — [3]Department of Physics, Sabang Sajanikanta Mahavidyalaya, Paschim Medinipur, India

Ultrathin NiO films have prospective applications especially in heterogeneous catalysis, microelectronics, and spintronics and are thus an object of active research. The Ag(100) surface is the usual support for these films, as its cubic lattice parameter is only 2.2 % smaller than that of NiO, which enables pseudomorphic growth at very low thicknesses. We have studied the NiO(100) surface for three thicknesses of the oxide: 2 ML on Ag(100), 20 ML on the same substrate, and a bulk single crystal. We have used intensity-voltage low-energy electron diffraction (IV-LEED) in combination with X-ray photoelectron spectroscopy (XPS) and density-functional theory (DFT) calculations. We focus on differences among the three thicknesses, mainly in terms of lattice parameters and surface defects, and our study deepens existing knowledge of the growth of ultrathin NiO films. The IV-LEED calculations have been carried out using the AQuaLEED package, which will also be briefly presented.

O 92.5 Fri 11:30 CHE 91

LEED I(V) with ViPErLEED: Overview and Applications — •Alexander M. Imre[1], Florian Kraushofer[1,2], Florian Doerr[1], Tilman Kisslinger[3], Michael Schmid[1], Ulrike Diebold[1], Lutz Hammer[3], and Michele Riva[1] — [1]TU Wien, Vienna, Austria — [2]TU Munich, Munich, Germany — [3]FAU Erlangen-Nürnberg, Erlangen, Germany

LEED $I(V)$ is an extension to qualitative Low Energy Electron Diffraction (LEED) pattern analysis in which diffraction intensities are quantitatively studied as a function of incident electron energy. This yields structural information about the surface that can be difficult to obtain otherwise. Regrettably, LEED $I(V)$ has been underutilized by the surface science community over the last decades.

Our group has developed the Vienna Package for TensErLEED (ViPErLEED); a suite of hardware and software aiming to drastically reduce the barrier of entry for the technique. The three core parts of ViPErLEED are: (1) electronics that enable upgrading existing LEED setups for LEED $I(V)$, (2) a spot tracker for easy $I(V)$ curve extraction, and (3) a Python package for LEED $I(V)$ analysis based on the TensErLEED package.

We present a quick overview of ViPErLEED and give insight into current developments. We then show LEED $I(V)$ results obtained and analyzed using ViPErLEED for the α-Fe_2O_3(012)-(1×1) and (2×1) surfaces. While a bulk-truncation is confirmed for α-Fe_2O_3(012)-(1×1), current structural models cannot explain the (2×1) termination.

O 92.6 Fri 11:45 CHE 91

Reduction by H2 exposure at room temperature of ceria ultrathin films grown by atomic layer deposition — •Carlos Morales, Yuliia Kosto, Rudi Tschammer, Karsten Henkel, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Konrad-Zuse-Strasse 1, D-03046 Cottbus, Germany

Atomic layer deposition (ALD) exhibits a high potential for integration as a scalable process in microelectronics, allowing well-controlled layer-by-layer deposition and conformal growth on 3D structures. Yet, the ALD technique is also well known to lead to amorphous and defective, non-stoichiometric films, potentially resulting in modified materials properties that, in the case of ultra-thin deposits, can also be affected by film/substrate interaction. Interestingly, initial in situ X-ray photoemission spectroscopy (XPS) measurements of ceria ALD-deposits on Al2O3/Si, sapphire, and SiO2 substrates confirm a Ce3+/Ce4+ mixture dependent on the substrate interaction, deposit thickness, and morphology. Using near-ambient pressure XPS, we have significantly reduced ultrathin (< 10 nm) ceria films grown by ALD by exposing them to different O2/H2 partial pressures at moderate temperatures (< 525K). Notably, the total amount of reduction to Ce3+ is found to depend on the deposit thickness and initial ceria/substrate interaction. Furthermore, the intrinsic defects related to the ALD method seem to play a critical role in the reversible reduction at room temperature.

O 92.7 Fri 12:00 CHE 91

Role of orientation and oxyhydroxide formation on the OER activity of LaNiO$_3$ surfaces — •Achim Füngerlings[1], Marcus Wohlgemuth[2], Marcel Risch[3], Felix Gunkel[2], Christoph Bäumer[2,4], and Rossitza Pentcheva[1] — [1]Department of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [2]Peter Gruenberg Institute and JARA-FIT, Forschungszentrum JuelichGmbH, Juelich, Germany — [3]Nachwuchsgruppe Gestaltung des Sauerstoffentwicklungsmechanismus, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [4]MESA+ Institute for Nanotechnology, Faculty of Science and Technology,University of Twente, Enschede, Netherlands

We present a combined experimental and theoretical study of the influence of surface orientation and transformation on the OER activity of Ni-terminated (001), (110) and (111) oriented LaNiO$_3$ films, epitaxially grown on SrTiO$_3$ substrates via pulsed laser deposition and characterized by AFM and XRD, as well as Hall measurements of the electrical conductivity. Cyclic voltammetry shows the lowest overpotential for (111) and the highest for (001), and gives indication for the formation of a surface oxyhydroxide(-like) skin layer, supported by EXAFS measurements. Based on density functional theory calculations with an on site Hubbard U, we explored different models for the transformed surfaces and find a strong sensitivity of the OER activity on interlayer H concentration and number of oxyhydroxide layers with distinct behavior of the two surface orientations.

O 92.8 Fri 12:15 CHE 91

Electron-phonon coupling for the 2D electron gas at EuO/KTaO$_3$(001) studied by HREELS — •Hannes Herrmann, Anne Oelschläger, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, 06120 Halle, Germany

Recent studies at the KTaO$_3$(111) surface revealed a 2D electron gas (2DEG) with much higher charge carrier density than in SrTiO$_3$-based heterostructures [1]. Similar 2DEGs with lower charge carrier densities could be obtained on the (011) and (001) surfaces [2].

In this work, we study surface plasmon polaritons (SPP) and their coupling to a 2DEG with high-resolution electron energy loss spectroscopy (HREELS). By evaporating Eu on top of KTaO$_3$(001), a 2DEG is initiated resulting in a pronounced asymmetric SPP line shape and extreme broadening compared to the phonons of the clean surface. The line shape will be analysed in terms of a strong coupling of the SPP with the 2DEG. The response can be described by a two-layer model with a 2D Drude-like response with frequency-dependent electronic mobility on top of a bulk-like KTaO$_3$.

[1] A. F. Santander-Syro, C. Bareille, F. Fortuna and M. J. Rozenberg, Phys.Rev. B 86, 121107 (2012)
[2] P. D. C. King, R. H. He, T. Eknapakul and W. Meevasana, Phys. Rev. Lett. 108.117602 (2012)

O 92.9 Fri 12:30 CHE 91

2D electron gas and interdiffusion processes at the EuO/SrTiO$_3$(001) interface — •Anne Oelschläger, Hannes Herrmann, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, 06120 Halle, Germany

The deposition of metallic europium (Eu) on SrTiO$_3$(001) (STO) creates a two-dimensional electron gas (2DEG) and concomitant Ti^{3+}-O$_2$-vacancy complexes [1]. Here we study this interface by HREELS, XPS and LEED. The phonon spectra are dominated by the dipole-active surface phonon polaritons of STO. They show a prominent broadening in the presence of the 2DEG due to strong electron-phonon coupling.

Upon annealing to 1020 K, the Ti^{3+} related photoemission lines as well as the phonon broadening vanish. We assign these changes to diffusion of oxygen from the bulk to the EuO/STO interface. Finally, the intensity ratio of Sr3p and Ti2p core levels indicates a diffusion of Ti to the europium oxide (EuO) layer, i.e. formation of EuTiO$_3$.

[1] P. Lömker et al. Phys. Rev. Mater. 1, 062001(R), 2017

O 92.10 Fri 12:45 CHE 91

Surface Structures of La$_{0.8}$Sr$_{0.2}$MnO$_3$(001): from Commensurate to Quasicrystal Phases — •Erik Rheinfrank[1], Michael Brunthaler[1], Giada Franceschi[1], Peter Matvija[2], Michael Schmid[1], Ulrike Diebold[1], and Michele Riva[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Faculty of Mathematics and Physics,Department of Surface and Plasma Science, Charles University, Prague, Czech Republic

Lanthanum-strontium manganite (La$_{0.8}$Sr$_{0.2}$MnO$_3$, LSMO) is a perovskite oxide used as a cathode material in solid oxide fuel cells, which convert chemical energy to electrical energy. To gain deeper insights into the reaction mechanisms, it is important to understand the structure of the surface at the atomic scale. To this end, we grow atomically flat single-crystalline LSMO(001) thin films on Nb-doped SrTiO$_3$ (STO) substrates via pulsed laser deposition (PLD). The as-grown films have a B-site (Mn) rich surface that can be transformed into an A-site (La/Sr) rich structure by Ar$^+$ sputtering and subsequent annealing. The B-site rich surface is recovered by depositing Mn from a MnO target. In low-energy electron diffraction (LEED), the Mn-rich surface shows a 4-fold symmetric structure that is best explained by a set of four basis vectors. This is reminiscent of quasicrystals. Scanning tunneling microscopy reveals a non-periodic structure with a Fourier transform consistent with the LEED pattern.

O 93: Graphene II: Electronic Structure and Growth

Time: Friday 10:30–12:30 Location: GER 37

O 93.1 Fri 10:30 GER 37

Energy dissipation on magic angle twisted bilayer graphene — •Marcin Kisiel, Alexina Ollier, Urs Gysin, and Ernst Meyer — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Understanding nanoscale energy dissipation is nowadays among few priorities particularly in quantum systems. While traditional Joule dissipation omnipresent in today's electronic devices is well understood, the energy loss of the strongly interacting electron systems remains largely unexplored. Twisted bilayer graphene (tBLG) is a host of interaction-driven correlated insulating phases, when the relative rotation is close to the magic angle (1.08deg). Here, we report on low temperature (5K) nanomechanical energy dissipation of tBLG measured by sharp tip of the pendulum atomic force microscope (pAFM). Ultrasensitive cantilever tip acting as an oscillating gate over the quantum device shows dissipation peaks attributed to different fractional filling of the flat energy bands. pAFM provides exquisite spatial resolution and thus allows to determine the twist angle distribution of tBLG. Strikingly it does it without literally touching the sample surface. Application of magnetic fields provoked strong oscillations of the dissipation signal at 3/4 band filling, which we identified as familiar to Aharonov-Bohm oscillations. The work demonstrates that nanomechanical energy dissipation provides a rich source of information on the dissipative nature of the correlated electronic system of tBLG, with implications for coupling a mechanical oscillator to the quantum devices.

O 93.2 Fri 10:45 GER 37

Raman features of graphene and weyl semimetals beyond the standard nonadiabatic theory — •Nina Girotto and Dino Novko — Institute of Physics, Zagreb, Croatia

Although graphene has already been thoroughly studied with Raman spectroscopy, there still exists a disagreement about the broadening mechanisms of the E2g mode and its actual temperature dependence [Nano Lett. 10, 466 (2010)]. Along with the importance of the nonadiabatic effects in graphene, higher order electron-phonon scattering processes also significantly impact the phonon spectrum. Specifically, the electron-phonon-induced lifetime and energy renormalization of the electron-hole pair excitations bring additional temperature dependence in the electron-coupled phonon modes and their corresponding linewidths. The nonadiabatic theory relying on first principles calculations, developed in [Phys. Rev. B 98, 041112(R) (2018)], is here successfully applied to graphene in various doping regimes and to Weyl semimetals, which contain a 3-dimensional analog of Dirac points in the electron band structure and are, therefore, excellent candidates for achieving a nonadiabatic regime.

O 93.3 Fri 11:00 GER 37

Near-field optical investigation of tetralayer graphene reveals ABCB stacking — •Konstantin G. Wirth[1], Jonas B. Hauck[2], Alexander Rothstein[3], Christoph Stampfer[3], Dante M. Kennes[2], Lutz Waldecker[3], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Institute for Theory of Statistical Physics, RWTH Aachen University — [3]2nd Institute of Physics, RWTH Aachen University

The crystallographic structure of few-layer graphene (FLG) greatly influences its electronic and optical properties. Local probing of the stacking order is usually done by optical measurements, such as infrared absorption [1] or Raman spectroscopy, which work for non-contacted and encapsulated samples but are limited in lateral resolution by diffraction to a few micrometer. Here, we directly probe the electronic properties of tetralayer graphene (4LG) with amplitude and phase-resolved near-field spectroscopy with a broadly tunable laser source over the energy range from 0.28 to 0.56 eV. We differentiate between rhombohedral and Bernal stacking sequences and reveal domains of the previously elusive third stacking order of 4LG, namely ABCB[2], by addressing distinctive interband contributions in optical conductivity. These results establish near-field spectroscopy at the interband transitions as a semi-quantitative tool, enabling the recognition and characterization of FLG domains.

[1] Mak et al., PNAS, 2010 107, 14999-15004 [2] Wirth et al., ACS Nano 2022, 16, 16617-16623

O 93.4 Fri 11:15 GER 37

Image potential states as local probes for graphene magnetism — •Maciej Bazarnik[1,2,3], Roland Wiesendanger[3], and Anika Schlenhoff[1] — [1]Institute of Physics, University of Münster, Germany — [2]Institute of Physics, Poznan University of Technology, Poland — [3]Department of Physics, University of Hamburg, Germany

Image-potential states (IPSs) evolving in front of polarizable surfaces are known to serve as quantum sensors for various properties, including surface magnetization and interfacial coupling at buried interfaces. Using a spin-polarized scanning tunneling microscopy (SP-STM) setup, the spin-polarized IPS can be probed locally. In hybrid systems such as iron (Fe) -intercalated graphene (Gr) on Ir(111), Fe is known to grow pseudomorphically on the Ir substrate in a monolayer thickness limit. In contrast, the Gr overlayer exhibits a substantial buckling within the moiré unit cell, resulting in a laterally varying hybridization to the Fe. As a result, the monolayer Gr exhibits a laterally varying spin-polarization within the moiré unit cell.

Here, we present resonant tunneling studies on Fe-intercalated Gr, showing a much stronger contrast between the fcc and hcp parts of the moiré unit cell compared to conventional STM images on this system. Moreover, our SP-STM studies show that the IPSs are sensitive to the interlayer coupling of Gr to the underlying ferromagnet. The resulting local IPS spin-polarization can be used to probe the atomic-scale magnetism within the moiré unit cell of the ferromagnet graphene hybrid system.

O 93.5 Fri 11:30 GER 37

Quantitative measurement and first principle prediction of the adsorption structure of graphene on Cu(111) — •Matthew A. Stoodley[1,2], Benedikt P. Klein[1,2], Luke A. Rochford[2], Tien-Lin Lee[2], David A. Duncan[2], and Reinhard J. Maurer[1] — [1]University of Warwick, Coventry, United Kingdom — [2]Diamond Light Source, Didcot, United Kingdom

Copper is the dominant substrate for the industrial scale growth of graphene, and graphene-functionalised copper foils are regularly employed as electrodes and heterogeneous catalysts. Yet, little is known about the structure of the graphene-copper interface. We report a quantitative measurement of the adsorption height of graphene on Cu(111) using the x-ray standing waves technique. Using state-of-the-art dispersion-corrected density functional theory, we tested different structural models of graphene on copper. Quantitative agreement with experiment could only be achieved by accounting for the moiré superstructure of the graphene layer on the copper surface. We further investigate how lattice strain affects long-range dispersion interactions and therefore the adsorption height of graphene on Cu(111) as well as graphene bilayer interlayer distances. We use these results to assess the predictive capabilities of common dispersion-corrected density functional approximations. Exploration of the adsorption energy of aromatic molecules of varying size, from benzene to graphene enables us to explore size effects between the substrate and organic overlayer.

O 93.6 Fri 11:45 GER 37

Determining the stability and catalytic formation of graphene on liquid Cu using machine-learning potentials — •Hao Gao[1], Valentina Belova[2], Maciej Jankowski[2], Hendrik H. Heenen[1], Gilles Renaud[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]ESRF, Grenoble, France

The rapid, high-quality synthesis of graphene (Gr) on liquid Cu catalysts is microscopically still poorly understood. This is due to the difficult characterization of the Cu liquid surface. Especially in atomistic simulations, the large length and time scales necessary to reliably emulate the temporal evolution of the liquid are a major challenge. Corresponding molecular dynamics simulations require large simulation cells and need to span well into the nanosecond regime – an endeavor presently intractable via first-principles methods. In this work we use computationally efficient machine-learning potentials (MLPs) trained to density-functional theory (DFT) data in order to extrapolate the first-principles predictive power to the required scales. Detailed benchmarking confirms that our MLP captures the involved physics well, accurately reproducing the experimentally determined Gr adsorption height. We apply the MLP to further obtain free energy barriers of possible rate-limiting steps which can be compared to the distinct reaction kinetics found experimentally. Our work draws a path for the use of reliably trained MLPs as a multiscale modeling technique to explore previously unchartered computational problems. In that we provide new insight into the domain of liquid metal catalysts which generally lack atomic-scale understanding.

O 93.7 Fri 12:00 GER 37

In-situ photoemission electron microscopy investigation of mono- and bilayer graphene growth on Ru($10\bar{1}0$) — •Lukas Schewe, Cathy Sulaiman, Lars Buss, Moritz Ewert, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg

Epitaxial graphene growth has often been studied on close-packed transition metal substrates, e. g., the Ru(0001) surface, which is a well-studied model system for strong graphene-support interaction. Here, we focus on a Ru surface with different symmetry, i. e., the Ru($10\bar{1}0$) surface, to investigate the influence of the presumably modified graphene-substrate interaction on the growth of epitaxial monolayer and bilayer graphene (MLG, BLG) islands. The structural and chemical differences of the graphene on the two different surfaces are investigated by photoemission electron microscopy (PEEM), delivering information on both morphology and electronic structure. In-situ PEEM observation of graphene growth on the Ru($10\bar{1}0$) substrate by ethylene decomposition reveals the growth characteristics of MLG and BLG, the latter showing second layer nucleation via surface segregation of carbon. Furthermore, depending on growth temperature and relative orientation of the growing islands and surface steps, different growth characteristics are observed, in contrast to previous studies of the graphene/Ru(0001) system whereas similar electronic properties seem to prevail. Yet, when the MLG is decoupled from the Ru($10\bar{1}0$) substrate via intercalation of oxygen a distinct shift in work function is identified, slightly different from the resulting shift on Ru(0001).

O 93.8 Fri 12:15 GER 37

Defective graphene by topological design — Benedikt P Klein[1,2], Matthew A Stoodley[1,2], Joel Deyerling[3], Michael Clarke[4], Luke A Rochford[1], Marc Walker[2], Raymundo Marcial Hernandez[5], Christian B Nielsen[5], Lars Sattler[6], Sebastian M Weber[6], Gerhard Hilt[6], Alexander Generalov[7], Alexei Preobrajenski[7], Leon BS Williams[1,8], Tien-Lin Lee[1], Alex Saywell[4], Willi Auwärter[3], Reinhard J Maurer[2], and •David A Duncan[1] — [1]Diamond Light Source, UK — [2]University of Warwick, UK — [3]Technische Universität München, Germany — [4]University of Nottingham, UK — [5]Queen Mary University of London, UK — [6]Carl von Ossietzky Universität Oldenburg, Germany — [7]MAX IV, Lund, Sweden — [8]University of Glasgow, UK

Defective graphene is a promising material for both applications in electronic devices and as substrates for modern catalysts. However, generating deliberate imperfection in graphene often relies on brute force methods, like ion sputtering. Herein, we demonstrate one-step bottom-up synthesis of defective graphene with incorporated 5- and 7-membered ring defects by using a polyaromatic feedstock that contains the same topology as the desired defect. Furthermore, the ratio of ideal to defective graphene could be controlled by the temperature used to grow the film. By a combination of X-ray standing waves, non-contact atomic force microscopy, X-ray photoelectron spectroscopy, near-edge X-ray absorption fine structure and density functional theory, we thoroughly characterise these networks and propose this method as a novel method of functionalising graphene.

O 94: Topology and Symmetry-Protected Materials

Time: Friday 10:30–13:00 Location: GER 38

O 94.1 Fri 10:30 GER 38

Multigap topology and non-Abelian braiding of phonons from first principles — •Bo Peng[1], Adrien Bouhon[1,2], Bartomeu Monserrat[1,3], and Robert-Jan Slager[1] — [1]TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]Nordic Institute for Theoretical Physics (Nordita), Stockholm University and KTH Royal Institute of Technology, Hannes Alfvéns väg 12, Stockholm SE-106 91, Sweden — [3]Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom

Non-Abelian braiding of quasiparticles can encode information immune from environmental noise with the potential to realize topological quantum computation. Here we propose that phonons, a bosonic excitation of lattice vibrations, can carry non-Abelian charges in their band structures that can be braided using external stimuli. Taking some earthly abundant materials such as silicates [1] and aluminium oxide [2] as representative examples, we demonstrate that an external electric field or electrostatic doping can give rise to phonon band inversions that induce the redistribution of non-Abelian charges, leading to non-Abelian braiding of phonons. We show that phonons can be a primary platform to study non-Abelian braiding in the reciprocal space, and we expand the toolset to study such braiding processes.

References: [1] Nature Communications 13, 423 (2022). [2] Physical Review B 105, 085115 (2022).

O 94.2 Fri 10:45 GER 38

Electronic Structure of the Weak 3D Topological Insulator $Bi_{12}Rh_3Ag_6I_9$ — •Johannes Hessdörfer[1,2], Eduardo Carillo-Aravena[2,3], Armando Consiglio[2,4], Maximilian Ünzelmann[1], Michael Ruck[2,3], Domenico Di Sante[5], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany — [3]Anorganische Chemie II, Technische Universität Dresden, Germany — [4]Theoretische Physik I, Universität Würzburg, Germany — [5]University of Bologna, Italy

Weak three-dimensional (3D) topological insulators (TI) can be considered as a stack of 2D TI separated by insulating spacer layers. The first experimentally observed weak TI is $Bi_{14}Rh_3I_9$ [1], in which the TI layers are Kagome nets formed by rhodium centered bismuth cubes. Importantly, a modification of the $[Bi_2I_8]^{2-}$ spacer layer, like e.g. by Ag-substitution, can change the coupling between the 2D-TI and with that decisively influences the topological properties. Here, we investigate $Bi_{12}Rh_3Ag_6I_9$ by means of angle-resolved photoemission experiments and density functional theory band structure calculations. In particular, we will discuss the influence of the modified spacer layer on the electronic structure and compare the results with $Bi_{14}Rh_3I_9$ and other compounds of this family.

[1]Rasche et al., Nat. Mater, 12, 422-425 (2013)

O 94.3 Fri 11:00 GER 38

Doping of coupled 1D topologically protected edge states on the (001) surface of the topological crystalline insulator (Pb,Sn)Se — •Florian Keller, Artem Odobesko, and Matthias Bode — Physikalisches Institut, Lehrstuhl für Experimentelle Physik II, Julius-Maximilians-Universität Würzburg, Würzburg, Germany

Topological crystalline insulators (TCI) are a class of materials with topological protected surface states protected by crystalline symmetry. One representative of this material class is (Pb,Sn)Se which exhibits Dirac fermions at the surface and topologically protected one-dimensional edge state at the step edges with a height equivalent to an odd number of atomic layers [1]. It was shown that the 1D edge states hybridize when two or more odd step edges are in close proximity [2]. The nature of this hybridization indicates that the quasiparticle edge mode is not an infinite quantum 1D state, but is either strongly localized or has a very short coherence length along the edge. One way to check this hypothesis is to increase the coherence length by shifting the Dirac energy close to the Fermi energy [3]. Here we present experiments where Fe adatoms are deposited onto p-doped PbSnSe, resulting in a downwards-bending of the surface band structure. The dependence of the correlation length of Dirac fermions is investigated by determining the edge state hybridization for pristine and doped (Pb,Sn)Se.

[1] P. Sessi *et al.*, Science **354**, 6317 (2016)
[2] J. Jung *et al.*, Phys. Rev. Lett. **126**, 236402 (2021)
[3] P. M. Echenique *et al.*, Surf. Sci. Rep. **52**, 219 (2004)

O 94.4 Fri 11:15 GER 38

Pressure-driven tunable properties of the small-gap chal-

copyrite topological quantum material ZnGeSb$_2$: A first-principles study — •Surasree Sadhukhan[1], Banasree Sadhukhan[2], and Sudipta Kanungo[1] — [1]Indian Institute of Technology Goa, 403401 Ponda, India — [2]KTH Royal Institute of Technology, Stockholm

Search for new topological quantum materials is the demand to achieve substantial growth topological phase of matter. In this search process, theoretical prediction is crucial besides the obvious experimental verification. The divination of topological properties in already well-known narrow gap semiconductors are flourishing in quantum material science. We revisited the semiconductor compound in the chalcopyrite series, some of which were potential topological materials. Using this density functional theory-based first-principles calculations, we report a strong topologically nontrivial phase in chalcopyrite ZnGeSb$_2$, which can act as a model system of strained HgTe. The estimates reveal the non-zero topological invariant (Z$_2$), Dirac cone crossing in the surface spectral functions with spin-momentum locked spin texture. We also report the tunable topological properties from nontrivial to trivial phases under moderate hydrostatic pressure within *7 GPa. A minor modification of a lattice parameter is enough to achieve this topological phase transition easily accomplished in an experimental lab. We have incorporated the discontinuity in the tetragonal distortion of non-centrosymmetric ZnGeSb$_2$ to drive the topological quantum phase transition.

O 94.5 Fri 11:30 GER 38

Shift current in the Haldane model: analytic and numerical evaluation — •Javier Sivianes Castaño and Julen Ibañez Azpiroz — Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain

The shift current is a second order optical response which takes place in noncentrosymmetic crystals and is characterized by a DC photocurrent. As realized recently, the shift current is sensitive to the topology of materials [1]. In particular, DFT calculations have predicted a sign change when going through a topological phase transition (TPT) in the bulk crystals BiTeI and CsPbI$_3$ [2]. Here we analyse the shift current in the Haldane model, as a toy model that describes inversion symmetry breaking and features non-trivial topological phases. We derive a simple analytical expression that accounts for the sign change across the TPT by relating it to the inversion of the mass term, in agreement with Ref [3]. We complement our study by a numerical evaluation on a continuum version on the Haldane model [4]. In this description we study the quantitative importance of the off-diagonal matrix elements of the position operator that are commonly discarded in the tight-binding description.

Funding provided by the European Union's Horizon 2020 research and innovation programme under the European Research Council (ERC) grant agreement No 946629.

[1] T. Morimoto and N. Nagaosa, Sci. Adv. **2**, 5 (2016) [2] L. Z. Tan and A. M. Rappe, PRL **116**, 237402 (2016) [3] Z. Yan, arXiv:1812.02191 [4] J. Ibañez-Azpiroz et al., PRB **92**, 195132 (2015)

O 94.6 Fri 11:45 GER 38

The 2D Ferromagnetic Extension of a Topological Insulator — •Philipp Kagerer[1,2], Celso I. Fornari[1,2], Sebastian Buchberger[1,2], Begmuhammet Geldiyev[1,2], Teresa Tschirner[2,3], Louis Veyrat[2,3,4], Abdul V. Tcakaev[2,4], Martin Kamp[5], Sergio L. Morelhao[6], Vladimir Hinkov[2,4], Hendrik Bentmann[1,2], and Friedrich Reinert[1,2] — [1]Exp. Physik VII, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Leibnitz IFW Dresden — [4]Exp. Physik IV, Universität Würzburg — [5]Physikalisches Institut and RCCM, Universität Würzburg — [6]Instituto de Física, Universidade de São Paulo

3D topological insulators (TI) are known to have a topological nontrivial band structure protected by time reversal symmetry, which also guarantees the metallicity of the surface. Consequently, it is sufficient to break this symmetry only locally at the surface of the sample to gap out the topological surface state (TSS), leading to a variety of novel topological effects, e.g. an axion term in the electromagnetic response and quantized spin-selective edge channels. While most experimental approaches to date have aimed to introduce magnetism globally, we present the first experimental realisation of the *ferromagnetic extension* (1), a design directly interfacing a 3D TI with a two-dimensional non-trivial magnet. Utilizing a single septuple layer MnBi$_2$Te$_4$ on the prototypical TI Bi$_2$Te$_3$, we establish a stable 2D ferromagnetic ground state and introduce a sizeable magnetic exchange gap in the TSS (2).
(1) M.M. Otrokov et al., 2D Mater. **4**, 025082 (2017)
(2) P. Kagerer et al., arXiv 2207.14421 (2022)

O 94.7 Fri 12:00 GER 38

Orbital angular momentum in indenene measured by circular dichroism in ARPES — •Jonas Erhardt, Cedric Schmitt, Simon Moser, and Ralph Claessen — Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg D- 97074, Germany

Indenene, a monolayer of In atoms arranged in a triangular lattice on SiC(0001), has recently been identified as a quantum spin Hall insulator (QSHI) [1]. Its topological character is encoded in a characteristic energy staggering of its orbital angular momentum (OAM) polarized Dirac states [1]. This makes indenene an ideal test case for recent claims that circular dichroism in angle-resolved photoelectron spectroscopy (CD-ARPES) gives access to local Berry curvature signatures via the OAM [2]. However, a particular challenge of such experiments is the extraction of the intrinsic OAM-related CD signal, requiring its distinction from final state effects and extrinsic contributions induced by experimental geometry.
In this talk, I will present a systematic photon energy dependent CD-ARPES study of indenene's Dirac states and use simple geometric considerations to disentangle experimental from OAM induced CD. The resulting OAM sequence confirms indenene to be a QSHI and thus establishes a new approach to experimentally identify the topological character of a 2D quantum material directly from its bulk states.

[1] M. Bauernfeind *et al.*, Nat. Commun., **12**, 5396 (2021)
[2] M. Schüler *et al.*, Sci. Adv., **6**, 2730 (2020)

O 94.8 Fri 12:15 GER 38

Transfer matrix analysis of non-Hermitian interfaces — •Jacob Fauman — Max Planck Institute for the Science of Light, Erlangen, Germany

Non-Hermitian systems exhibit unique features not present in Hermitian systems, including the so-called non-Hermitian skin effect in which the modes accumulate at the surface of the system. We analyze the interface between a non-Hermitian system and a Weyl semimetal analytically using the transfer matrix method. This approach is especially well-suited to the study of spatially inhomogeneous systems, and allows for analysis of the Fermi arcs at the interface. We also consider the effect of Hermitian and non-Hermitian spectral degeneracies on the interface modes.

O 94.9 Fri 12:30 GER 38

Spectroscopic signatures of non-trivial topology in Weyl semimetals — •Jakub Schusser[1], Hendrik Bentmann[2], Maximilian Ünzelmann[1], Tim Figgemeier[1], Chul-Hee Min[3], Simon K. Moser[4], Jennifer N. Neu[5], Theo Siegrist[6], and Friedrich Reinert[1] — [1]Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, JMU Würzburg — [2]Center for Quantum Spintronics, NTNU Trondheim — [3]Department of Physics, CAU zu Kiel — [4]Exp. Physik IV and Würzburg-Dresden Cluster of Excellence ct.qmat, JMU Würzburg — [5]National High Magnetic Field Laboratory, Tallahassee, Florida — [6]Department of Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, Tallahassee, Florida

By performing angle-resolved photoemission spectroscopy (ARPES) on bulk samples we show the spectroscopic manifestation of topological features and Weyl physics beyond the simple photointensity over a broad range of excitation energies from the vacuum ultraviolet to the soft X-Ray regime and compare the surface to the bulk band structure. Our experimental observations were complemented by state-of-the-art first principle photoemission calculations based on one-step model of photoemission. The determinant criterion confirms the arc character of the spoon features in the constant energy contour close to Fermi level in non-centrosymmetric TaP. We further show the drawbacks of the existing spectroscopic techniques used to determine whether the given material has non-zero Chern number and discuss an improved approach for identifying Fermi arcs by the means of differential ARPES measurements as well as the proper final state description.

O 94.10 Fri 12:45 GER 38

Extended Hatano-Nelson model, exceptional points and spectral symmetry — •Julius Gohsrich[1,2], Sharareh Sayyad[1], and Flore K. Kunst[1] — [1]Max Planck Institute for the Science of Light, Staudtstraße 2, 91058 Erlangen, Germany — [2]Department of Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Non-Hermitian systems attract a lot of attention in recent years as effective description of open quantum systems. A prominent example in this context is the Hatano-Nelson model. While historically the model has short-range non-reciprocal hoppings, long-range hopping has not been systematically studied. In this talk, I will present our results on the extended Hatano-Nelson model. Using analytical techniques, we demonstrate how the underlying physics of the original Hatano-Nelson model is enriched when longer-range hoppings are also included. I will discuss how the crucial elements of the Hatano-Nelson model, namely, the non-Hermitian skin effect and the exceptional points, are modified for the generalized model.

O 95: Focus Session: Making Experimental Data F.A.I.R. – New Concepts for Research Data Management II (joint session O/TT)

Time: Friday 9:30–12:45 Location: WIL A317

Topical Talk O 95.1 Fri 9:30 WIL A317

FAIRifying ARPES: a Route to Open Data & Data Analytics — •Ralph Ernstorfer[1,2], Tommaso Pincelli[1,2], Patrick R. Xian[2], Abeer Arora[2], Florian Dobener[3], Sandor Brockhauser[3], and Laurenz Rettig[2] — [1]TU Berlin, Germany — [2]Fritz-Haber-Institut Berlin, Germany — [3]HU Berlin, Germany

While angle-resolved photoemission spectroscopy (ARPES) is the most direct probe of crystals' electronic structure, the globally collected ARPES data have not been merged into an open experimental electronic structure database in equivalence to well-established atomic structure databases. We discuss a data format based on NeXus [1] as a concept for unifying the data structure for all types of photoemission experiments including time-, spin-, and time-resolved ARPES [2]. The aim is to immediately enable preprocessed data and metadata shareability according to FAIR data principles, employing existing public storage and archiving research data infrastructures such as Zenodo, OpenAIRE, and Nomad/FAIRmat. Ultimately, the multidimensional photoemission spectroscopy (MPES) format is designed to allow high-performance automated access, providing experimental databases for high-throughput material search [3]. References: [1] https://www.nexusformat.org/ [2] https://mpes.science/; https://fairmat-experimental.github.io/nexus-fairmat-proposal/ [3] R. P. Xian et al., Scientific Data 7, 442 (2020); R.P. Xian et al., Nat. Comp. Sci, in print, arXiv:2005.10210

O 95.2 Fri 10:00 WIL A317

A FAIR data infrastucture for photoemission experiments — •Marten Wiehn[1], Tobias Eul[1], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Recent trends toward data-driven, high-tech experimental research and the growing volumes of data associated with it show the increasing importance of comprehensive data acquisition and management. We present an automated workflow for well-described photoemission data from experiment to archive and publication. Utilizing a powerful experiment control software to capture essential metadata for each measurement enables the collection of FAIR-ready data (Findable, Accessible, Interoperable, Reusable). In addition, using an electronic lab notebook pushes our lab further toward a FAIR data infrastructure that supports researchers in their daily work.

O 95.3 Fri 10:15 WIL A317

Multi-Dimensional Photoemission Spectroscopy: a concept for FAIR photoemission data — •Florian Dobener[1], Tommaso Pincelli[2,3], Abeer Arora[2,4], Steinn Ymir Augustsson[5], Dmytro Kutnyakhov[6], Michael Hartelt[7], Laurenz Rettig[1], Martin Aeschlimann[2], Ralph Ernstorfer[7], and Sandor Brockhauser[2,3] — [1]Department of Physics, HU Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Institut für Optik und Atomare Physik, TU Berlin, Germany — [4]FU Berlin, Fachbereich Physik, Berlin, Germany — [5]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [6]DESY, Hamburg, Germany — [7]Department of Physics and OPTIMAS, University of Kaiserslautern, Germany

The complexity and size of photoemission data is rapidly increasing as new technological breakthroughs have enabled multidimensional parallel acquisition. However, most of the community is currently using heterogeneous data formats and workflows. We propose a new data format based on NeXus, a hierarchically organized hdf5 structure. This multidimensional photoemission spectroscopy format is designed to allow high-performance automated access, enabling experimental databases for high-throughput material search. Our approach involves reaching out to the community using a website with extensive documentation of our proposed standard. As a demonstrator of the potential of our approach we present a workflow and data pipeline integrated into the NOMAD research data management solution, which provides powerful analysis and search functionalities.

O 95.4 Fri 10:30 WIL A317

Towards an Infrastructure for FAIR Synthesis Data — •Sebastian Brückner[1,2], Andrea Albino[1], Jose Marquez[1], Florian Dobener[1], Hampus Näsström[1], Markus Scheidgen[1], Claudia Draxl[1], and Martin Albrecht[2] — [1]HU Berlin, Zum Großen Windkanal 2, 12489 Berlin — [2]IKZ Berlin, Max-Born-Straße 2, 12489 Berlin

A data infrastructure based on the FAIR (findable, accessible, interoperable and reusable) principles promises a new way of sharing and exploring data by using highly efficient data analysis and artificial intelligence tools. This also applies to data related to sample synthesis. At present, most synthesis data are not structured comprehensively or not even stored digitally but in handwritten lab books. There hardly exists any data standards in synthesis, which is in contrast to data from characterization techniques. The FAIRmat project (https://FAIRmat-NFDI.eu) is building a FAIR data infrastructure for condensed-matter physics and the chemical physics of solids. In FAIRmat's Area A, we focus on synthesis data to make sample synthesis reproducible, accelerate the development of novel materials, and make characterization data of synthesized materials assessable. Here we summarize our ongoing work and progress including: providing a general data model for synthesis which is harmonized with data from measurements and theory (ontologies); implementation of our data model in use cases and electronic laboratory notebooks; developing tools for data acquisition and analysis; data governance guidelines to enable a sustainable change of research data management at the institute/university level.

O 95.5 Fri 10:45 WIL A317

FAIRifying Material Synthesis with the NOMAD Electronic Laboratory Notebook (ELN) — •Andrea Albino[1], Hampus Näsström[1], Florian Dobener[1], Jose Marquez Prieto[1], Lauri Himanen[1], David Sikter[1], Mohammad Nakhaee[1], Amir Golparvar[1], Sebastian Brückner[1], Martin Albrecht[2], Markus Scheidgen[1], and Claudia Draxl[1,3] — [1]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany. — [2]Leibniz-Institut für Kristallzüchtung, Berlin, Germany. — [3]The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Berlin, Germany.

Approaching the era of big data-driven materials science, one crucial step to collecting, describing, and sharing experimental data is the adoption of ELNs. The project FAIRmat (fairmat-nfdi.eu) is offering such tools by developing and operating the open-source software NOMAD. The NOMAD ELN aims at offering a secure environment to protect the integrity of both data and metadata, whilst also affording the flexibility to adopt new synthetic processes or changes to existing ones without recourse to further software development.

We find that to promote an early adoption, it is important to adapt to a single user's needs and workflows. An inductive approach, going from a particular set of experiments to a general description of the similarities recurring in each of them, led us to adopt a common data structure as a standard. The state-of-the-art ELN features for a synthetic process will be shown in the talk, highlighting the development of both data modeling and specific implementation solutions.

O 95.6 Fri 11:00 WIL A317

FAIR Data Infrastructure for Computation: Classical Simulations and Multiscale Modeling — •Joseph F. Rudzinski[1,2], José M. Pizarro[1], Nathan Daelman[1], Luca M. Ghiringhelli[1], Karsten Reuter[3], Kurt Kremer[2], Silvana Botti[4], and Claudia Draxl[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Max-Planck-Institut für Polymer Forschung, Mainz — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [4]Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena

The emergence of the (big-)data-centric techniques as a fundamental paradigm of science calls for the development of infrastructure for ensuring FAIR—findable, accessible, interoperable, reusable—data management. The FAIRmat consortium aims to build extensive infrastructure for a wide variety of materials-science data, including soft matter simulations [1], by expanding upon the success of the NOMAD Laboratory—a repository for atomistic calculations in materials science [2]. Both the large volume and heterogeneous nature of classical molecular-dynamics simulation data presents a number of distinct challenges. In this talk, we present FAIRmat's progress in developing infrastructure for molecular-dynamics simulations, including metadata for molecular topologies and tools for workflow management. We will also discuss the need for standardization of metadata schemas and ontologies within the community, and planned collaborations with other open science initiatives and software developers.

[1] Scheffler, M. et al. Nature 2022, 604, 635-642.

[2] Draxl, C.; Scheffler, M. JPhys Materials 2019, 2, 036001.

Topical Talk O 95.7 Fri 11:15 WIL A317

Electronic Lab Notebooks in Teaching and Implications on Science — •Michael Krieger — Lehrstuhl für Angewandte Physik, Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

In our department, we have recently introduced Electronic Lab Notebooks (ELN) in the obligatory electronic lab course in the 4th semester of the physics curriculum. Immediate advantages for the students are obvious: all data, raw data and metadata including experiment description and experimental observations, are digitally stored at the same place. Moreover, student teams share and actively work in their group ELN with access at the university as well as at home, and script-based evaluations can be performed directly in the ELN.

The introduction of ELNs in teaching has also implications on science. Students carry their ELN experience and data competences into all research groups. There, however, modern research data management is much more complex. According to the FAIR principles, it requires structured, machine-readable data using open formats and vocabularies that meet community standards. The development of such standards is in many cases still to be done and is the core of the Nationale Forschungsdateninfrastruktur (NFDI). Here, ELNs in teaching provide a sandbox with short learning and innovation cycles for testing structured schemas. The experience helps to develop and establish sustainable and FAIR documentation of research workflows in science.

O 95.8 Fri 11:45 WIL A317

A step towards predicting synthesis conditions of metal-organic frameworks — •Dinga Wonanke[1], Thomas Heine[2], and Christof Wöll[1] — [1]Institut für Funktionelle Grenzflächen (IFG), Karlsruher , Germany — [2]Faculty of Chemistry and Food Chemistry,Dresden, Germany

The process of synthesising metal-organic frameworks (MOFs) falls under a branch of chemistry known as reticular chemistry. Here, well defined crystalline compounds are synthesised from a well thought out design principle by linking predefined building blocks under specific conditions. Although, this approach appears to be intuitive, the synthesis of any novel MOF still follows the conventional approach that begins with a thorough literature survey to explore reagents, calculations of aliquots and finally a series of time consuming and stressful trial-and-error syntheses. Consequently, although millions of stable hypothetical MOFs with interesting properties have been predicted, only approximately 100 thousand crystal structures of MOFs currently exist in the Cambridge Structural Database (CSD). Indicating a significant bottleneck in the intelligent design of novel stable MOFs with targeted properties.

In this talk, we will present an overview of our journey to design a new machine learning algorithm for predicting the synthesis condition of existing and hypothetical MOFs. We will discuss our experiences and challenges in mining and curating the MOF subset in the CSD. Finally, we will present our new MOF database that maps every MOF to its experimental synthetic conditions.

O 95.9 Fri 12:00 WIL A317

Deep learning surface scattering data analysis for processing large synchrotron datasets — •Vladimir Starostin, Valentin Munteanu, Linus Pithan, Alexander Gerlach, Alexander Hinderhofer, and Frank Schreiber — Institute of Applied Physics, University of Tübingen, Germany

In situ real-time surface scattering experiments such as grazing-incidence wide-angle X-ray scattering (GIWAXS) produce large amounts of data, frequently exceeding the capabilities of traditional data processing methods. Here we demonstrate an automated pipeline for the analysis of GIWAXS images, based on a machine learning architecture for object detection, designed to conform to the specifics of the scattering data [1]. Our pipeline enables real-time GIWAXS analysis and is designed to be employed at synchrotron facilities. We also present FAIR data strategies and traceable data resources from the raw data to the corresponding scientific publication and vice versa [2] including intermediate processing steps.

We demonstrate our method on real-time tracking of lead halide perovskite structure crystallization processes, which are relevant for hybrid solar cell applications. However, our approach is equally suitable for other crystalline thin-film materials by design. In general, the solution substantially accelerates the analysis process of GIWAXS images, potentially boosting the speed of scientific discoveries in material science.

[1] V. Starostin et al. *npj Comput Mater* **8**, 101 (2022)

[2] V. Starostin et al. *Synch Rad News* **13**, 31–37 (2022)

O 95.10 Fri 12:15 WIL A317

FAIR Data Infrastructure for Computation: Mapping out the Space of Density Functionals — •Nathan Daelman[1], Joseph F. Rudzinski[1,2], José M. Pizarro[1], Luca M. Ghiringhelli[1], Miguel A. L. Marques[3], Silvana Botti[4], and Claudia Draxl[1] — [1]Institut für Physik und IRIS-Adlershof, Humboldt-Universität zu Berlin, Berlin — [2]Max-Planck-Institut für Polymer Forschung, Mainz — [3]Institut für Physik, Martin-Luther-University Halle-Wittenberg, Halle — [4]Friedrich Schiller Universität Jena, Jena

The NOMAD Laboratory [1] holds over 135 million computational results, the vast majority of which stem from density-functional theory (DFT). The platform provides adequate querying and data analytics tools (e.g., machine-learning modelling) for processing such Big Data. However, the exchange-correlation (xc) functional with which the data was generated, limits the analysis scope of most thermodynamic and kinetic properties. Here, we present a strategy rooted in semantics for extending method interoperability. We will showcase our map of the entire xc-functional space that, in the context of the FAIRmat consortium [2], is built to be widely accessible and facilitate findability. Lastly, we will discuss the integration of this xc-functionals map into the NOMAD data platform, as well as its publication in ontology format as an effort towards a community-wide vocabulary standard.

[1] C. Draxl and M. Scheffler, MRS Bulletin 43, 676-682 (2018).

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

O 95.11 Fri 12:30 WIL A317

OpenSemanticLab: Towards Open Semantic Research — •Simon Stier and Matthias A. Popp — Fraunhofer ISC, Neunerplatz 2, 97082 Würzburg, Germany

In materials science, complex relationships exist between the properties of materials and their composition and processing. Therefore, digital transformation and acceleration in this domain represents a particularly important challenge. Although it is generally agreed that data must be linked by means of semantics and ontologies to form holistic data spaces, there is still a lack of suitable tools for integrating the necessary structures into the everyday work of scientists.

Fraunhofer ISC addresses this challenge with a broad-based strategy that closely links activities at all relevant levels. The goal hereby is the development towards Lab 4.0, the machine-readable documentation of scientific processes and the harmonization of data structures in accordance with international standards.

Core of the resulting OpenSource solution architecture is the central web data platform OpenSemanticLab [1] that links people (knowledge), machines (data) and algorithms (AI) equally. As an open system, this platform is easily adaptable even without programming knowledge and without losing the uniform structure. In this way, OpenSemanticLab enables us as scientists to contribute individually and yet in a standardized fashion to future digital materials research.

[1] https://github.com/OpenSemanticLab

O 96: Solid-Liquid Interfaces III: Reactions and Electrochemistry II

Time: Friday 10:30–13:00 Location: TRE Phy

O 96.1 Fri 10:30 TRE Phy

First step of the oxygen reduction reaction on Au(111): A computational study of the electrified metal/water interface — •Elias Diesen, Alexandra M. Dudzinski, Hendrik H. Heenen, Vanessa J. Bukas, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

While significant insight has been gained in recent years by first-principles simulations of electrochemical processes, crucial methodological challenges remain, especially for accurate determination of reaction energies under operando conditions. One open question is how to represent the constant electrode potential in simulations of an electrified water/metal interface, where the periodic simulation setup requires a constant charge in the simulation cell throughout the reaction. Here we compare different levels of treatment of the electrochemical interface: explicit *ab initio* molecular dynamics, an implicit solvent model, and a sawtooth-potential electric field in vacuum, for the case of O_2 adsorption on Au(111). We find that all methods agree qualitatively in predicting significantly enhanced O_2 binding at more reducing conditions. Important quantitative differences, however, are also presented and discussed. Umbrella sampling simulations shed light on the underlying free-energy landscape at varying potentials, while assessing the level of detail required in first-principles models of the electric double layer.

O 96.2 Fri 10:45 TRE Phy

Multiscale simulation of nanostructured electrocatalytic systems by coupling neural network surrogates and continuum models — •Younes Hassani Abdollahi[1,2], Jürgen Fuhrmann[3], and Sebastian Matera[1,2] — [1]Institut f. Mathematik, Freie Universität Berlin, Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [3]Weierstraß-Institut f. Angewandte Analysis u. Stochastik, Berlin, Germany

The kinetic Monte Carlo method (kMC) is the physically most sound approach for addressing the kinetic interplay of elementary processes at electrocatalytic surfaces but also comes at high computational costs. Therefore, computationally efficient surrogate models are highly desirable which allow the utilization of kMC simulation results in coarser scale simulations.

Using the oxygen reduction reaction on Pt(111) as a prototypical example, we investigate regression neural networks as surrogates to reproduce the stationary TOF as a function of all reaction conditions, i.e. electrostatic potential, concentrations, and temperature. We found that a relatively shallow network serves as an appropriate choice. This surrogate is then coupled to a conservative and thermodynamically consistent Finite Volume discretization of a nanofluidic model. The resulting hybrid mesoscale model will be employed to discuss the interplay of the nanostructure, transport, and kinetics.

O 96.3 Fri 11:00 TRE Phy

Modeling Transport Effects on Selectivity in Electrochemical CO_2 Reduction — •Hendrik H. Heenen[1,2], Georg Kastlunger[2], Vanessa J. Bukas[1], Karsten Reuter[1], and Karen Chan[2] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Technical University of Denmark, Lyngby, Denmark

Product selectivity in the electrochemical CO_2 reduction reaction (eCO_2RR) is known to change considerably with non-obvious parameters such as catalyst morphology or reactor design. In this work we explore the proposition that these parameters are related to selectivity through transport mediated desorption and adsorption of key intermediates. The mesoscopic morphology of a catalyst can be characterized by a measurable loading or roughness which determines the so-called active surface area. This area may in turn determine the selectivity by controlling the fate of desorbing (closed shell) intermediates along the reaction path: either to re-adsorb and further react on the surface, or to entirely leave the catalyst surface and form an early not fully-reduced product. We specifically show this competition in the reaction toward acetate which we propose to be governed by a solution reaction. Combining *ab initio* energetics, microkinetic and transport modeling in a multi-scale approach, we predict complex selectivity toward acetate with almost quantitative agreement to experiment. Finally, we demonstrate that the same principle applies to other important intermediates in the eCO_2RR. Mesoscopic transport thus provides an alternative or, at least, complementary explanation to changes in selectivity that are otherwise attributed to active sites changes, to doping, or to alloying.

O 96.4 Fri 11:15 TRE Phy

Kinetics of the initial step in Pt electrochemical oxidation — Jan Ole Fehrs[1], Timo Fuchs[1], •Olaf Magnussen[1], Chentian Yuan[2], David Harrington[2], Valentin Briega Martos[3], Serhiy Cherevko[3], and Jakub Drnec[4] — [1]Christian-Albrechts Universität zu Kiel — [2]University of Victoria — [3]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy — [4]European Synchrotron Radiation Facility

A key event in electrochemical metal oxidation is extraction of a metal atom from its lattice site to a location in a growing oxide. The direct observation of this fundamental step is difficult for base metals that actively corrode, because of the difficulty of producing clean surfaces and the speed of the oxidation. However, use of noble metals allows preparation of clean surfaces that are well-defined on the atomic scale, and for which in situ methods can directly observe this extraction. Here we show by fast simultaneous electrochemical and high-energy surface X-ray diffraction measurements, performed at the ID31 beamline of the European Synchrotron Radiation Facility with a photon energy of 70 keV, that the initial extraction of Pt atoms from Pt(111) is a fast, potential-driven process whereas charge transfer for the related formation of adsorbed oxygen occurs on a slower time scale. Electrochemical oxidation is therefore inherently different from gas-phase thermal oxidation, where the extraction must be driven by the chemisorption of oxygen species on the surface.

The work was funded by the Deutsche Forschungsgemeinschaft via grant 418603497 and the BMBF via project 05K19FK3.

O 96.5 Fri 11:30 TRE Phy

CO oxidation on Pt layers on Ru(0001): A UHV-STM, DEMS, and SXRD study — •Albert K. Engstfeld[1], Lukas Forschner[1], Mario Löw[2], Zenonas Jusys[2], Joachim Bansmann[2], R. Jürgen Behm[2], and Jakub Drnec[3] — [1]Ulm University, Institute of Electrochemistry, D-89069 Ulm — [2]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm — [3]ESRF, F-38000 Grenoble

According to the Sabatier principle, the performance of an (electro)catalyst material is determined by the fine balance between the binding strength of the reactants, reaction intermediates, and products to the catalyst surface. By changing the structural properties of the substrate, the electronic structure and in turn, also the binding of the species can be modified to tune the performance of the catalyst material. However, also the electrode‘s stability plays a crucial role in assessing the catalyst‘s performance.

Here we present results on the CO (and MeOH) electrooxidation on Pt layers with different thicknesses deposited on Ru(0001) under UHV conditions. The structural properties are studied by means of STM under UHV conditions before and after the electrochemical measurements. The electrocatalytic properties are studied in a flow cell (in a DEMS configuration) attached to the UHV chamber. This approach allows for disentangling surface redox processes from catalytic processes. Additional SXRD measurements provide additional insights into the stability of the electrodes. In combination, we discuss the fine balance between surface reactivity and electrode stability.

O 96.6 Fri 11:45 TRE Phy

Electrochemical Roughening of Stepped Platinum Surfaces — •Francesc Valls Mascaró[1], Marc Koper[1], and Marcel Rost[2] — [1]Leiden Institute of Chemistry, Leiden University — [2]Huygens-Kamerlingh Onnes Laboratory, Leiden Institute of Physics, Leiden University

Platinum is the model catalyst to be used in electrochemical energy conversion devices due to its high activity. Nevertheless, its industrial applicability is limited, as it degradates during fuel cell operation. This has been extensively studied by Cyclic Voltammetry and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) [1, 2]. It is well known that this degradation is linked to the nucleation and growth of platinum nanoislands on initially atomically flat terraces [3, 4, 5, 6]. However, there is no insight yet on the role of steps on this roughening process. In this work, we combine Cyclic Voltammetry and Electrochemical Scanning Tunneling Microscopy to study the stability of different stepped platinum surfaces upon oxidation-reduction cycling. Surprisingly, the electrochemical results indicate that neither 2D nor 3D (for Pt(533)) and no 3D (for Pt(553)) roughness develops, although we clearly observe island formation in the STM, and thus an increase in the step lengths and roughness.

[1] Topalov, A. et al., Chem. Sci., 5, 631 (2014) [2] Sandbeck D. J. S. et al., ACS Appl. Mater. Interfaces, 12, 25718 (2020) [3] Jacobse, L. et al., Nat. Mater. 17, 277 (2018) [4] Jacobse, L. et al., ACS Cent. Sci. 5 (12), 1920 (2019) [5] Rost, M. J. et al., Nat. Commun. 10, 5233 (2019) [6] Ruge, M. et al., J. Am. Chem. Soc., 139, 4532 (2017)

O 96.7 Fri 12:00 TRE Phy

Shaping the electrochemical interfaces of high-performance photoelectrodes by dedicated corrosion — •Matthias M. May[1,2], Erica A. Schmitt[1,2], Margot Guidat[1,2], Mario Löw[2], Anna-Lena Renz[1], Marco Flieg[1], Max Nusshör[1], Vibhav Yadav[1], Jongmin Kim[1], and Moritz Kölbach[1] — [1]Universität Tübingen, Institute of Physical and Theoretical Chemistry, Tübingen, Germany — [2]Universität Ulm, Institute of Theoretical Chemistry, Ulm, Germany

Photoelectrodes for highly efficient solar water splitting often involve III-V semiconductors, which exhibit only a limited stability under operating conditions due to (electro)chemical corrosion. Yet photoelectrochemical *in situ* functionalisation, which also involves dedicated corrosion, can effectively create an interphase that passivates the solid-liquid interface in a similar manner as solid-electrolyte interphases in batteries [1].

We show how this approach can be used to also electronically passivate III-V/Si dual junction photoelectrodes. A full understanding of the underlying photoelectrochemistry is, however, not yet achieved. To improve this understanding, we study the structural evolution of the interface in the electrolyte, using *operando* reflection anisotropy [2], improving the control of functionalisation and catalyst photoelectrodeposition.

[1] May and Jaegermann, Curr. Opin. Electrochem. **34** (2022) DOI:10.1016/j.coelec.2022.100968. [2] Löw et al., RSC Adv. **12** (2022) DOI:10.1039/D2RA05159A.

O 96.8 Fri 12:15 TRE Phy

Understanding the Interfacial Capacitance of 2D Materials in an Implicit Water Environment — •Hedda Oschinski[1,2], Karsten Reuter[1], and Nicolas G. Hörmann[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Technical University of Munich, Munich, Germany

The interfacial capacitance (C) is a central quantity in electrochemistry. For metal electrodes, C is dominated by the double layer capacitance that derives from the potential drop in the solvent. However, the finite density of states (DOS) in semiconducting 2D electrodes alters the picture and leads to a vanishing C around the point of zero charge. This entails a challenge in describing the energy-potential relation and the connected field effects when considering adsorbates. To explore this challenge, we study the interfacial capacitance for 2D metal halides MX_2, using density-functional theory in a continuum solvent environment. We break down C into a DOS-filling-related quantum capacitance and the double layer capacitance. Our analysis demonstrates that such a separation into individual components is not straightforward. Nevertheless, the qualitative behavior of C can be rationalized, making this study a first step towards better understanding of 2D, in particular semiconducting, electrodes.

O 96.9 Fri 12:30 TRE Phy

Initial Stages of Cathodic Corrosion of Au(111) in an Ionic Liquid — •Maren-Kathrin Heubach[1], Fabian M. Schuett[1], Areeg Abdelrahman[1], Ludwig A. Kibler[1], and Timo Jacob[1,2,3] — [1]Institute of Electrochemistry, Ulm University, Ulm, Germany. — [2]Helmholtz-Institute-Ulm (HIU), Ulm, Germany. — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany.

At potentials negative of 0 V *vs.* SHE, noble metal surfaces can be etched by a phenomenon called 'cathodic corrosion'.[1] For this process, absence of protons and presence of stabilising cations and adsorbed hydrogen at the electrode-electrolyte interface are required.[2] Even if the presence of water plays an important role,[3] in non-aqueous electrolytes such as ionic liquids, cathodic corrosion can take place as well.[4]

In this study, the cathodic corrosion of Au(111) in the hydrophobic ionic liquid *N*-methyl-*N*-propylpiperidinium bis(trifluoromethanesulfonyl)imide ([MPPip][TFSI]) was studied by *in situ* scanning tunnelling microscopy. Hereby, the formation of equidistant holes at the so-called 'elbows' of the Au(111) herringbone reconstruction was observed. Additionally, it was found that the water content plays a crucial role in the corrosion potential and extent. The higher the water content, the less negative is the onset potential of the cathodic corrosion and the more pits are formed at this potential.

[1] T. J. P. Hersbach, *et al.* Curr. Opin. Electrochem. **2021**, *26*, 100653. [2] A. I. Yanson, *et al.* Angew. Chemie Int. Ed. **2011**, *50*, 6346-6350. [3] M. M. Elnagar, *et al.* Electrochem. Sci. Adv. **2021**, e2100175. [4] F. Lu, *et al.* RSC Adv. **2013**, *3*, 18791.

O 96.10 Fri 12:45 TRE Phy

Parameters Determining Electrode Modification by High Voltage Electrolysis — •Lukas Forschner, Evelyn Artmann, Timo Jacob, and Albert K. Engstfeld — Institute of Electrochemistry, Ulm University, Ulm, Germany

Applying a sufficiently high voltage between two gas-evolving electrodes of different sizes in an aqueous electrolyte can lead to transition from normal electrolysis (NE) to Contact Glow Discharge Electrolysis (CGDE). Due to Joule heating, the electrolyte temperature increases significantly until enough solvent evaporates to form a stable gas sheath around the smaller electrode in which a plasma is ignited. Both in the NE and the CGDE region, the electrode surface can be altered significantly, e.g., by the formation of a Au oxide film[1] or nanoparticles.[2]

During high voltage electrolysis, there are several factors which could influence the restructuring of an electrode surface. First, to disentangle these processes, we measured the distribution of the electric potential in the electrolyte during NE using reversible hydrogen reference electrodes.[3] We found, supported by a COMSOL® model, that the potential distribution mainly depends on the electrolyte conductivity and the cell geometry. Furthermore, we show that the amount of Au oxide formed on a Au electrode during NE is more closely correlated to the current (density) than the voltage (usually provided in the literature).

[1] Artmann et al., *ChemPhysChem* **22** (2021) 2429. [2] Allagui et al., *Electrochim. Acta* **93** (2013) 137. [3] Forschner et al., (2022, submitted).

O 97: Focus Session: Scanning Probe Microscopy with Quartz Sensors IV

Time: Friday 10:30–12:45 Location: TRE Ma

O 97.1 Fri 10:30 TRE Ma

qPlus-based Lateral Force Microscopy — •Alfred J. Weymouth — Universität Regensburg, Regensburg, Deutschland

Lateral force microscopy (LFM) is a branch of AFM in which a component of force perpendicular to the surface normal is measured. Long-range forces have no lateral component over a flat terrace, making LFM ideal to study short-range forces. We have established methods to extract force and potential energy from our observations, and applied these methods to study a number of systems including molecular bending. We have also studied the interaction at the side of a molecular adsorbate, and more recently shown that we can measure the energy dissipation as we pull a molecule at the tip over the surface.

Giessibl et al., Proc. Nat. Acad. Sci. 99, 12006 (2002); Weymouth et al., Science 343, 1120 (2014); Weymouth, J Phys.: Condens. Matter 29, 323001 (2017); Weymouth et al., Phys. Rev. Lett. 124, 196101(2020); Weymouth et al, J. Jap. Appl. Phys. 61, SL0801 (2022)

O 97.2 Fri 10:45 TRE Ma

Exploring in-plane interactions beside an adsorbed molecule — •Shinjae Nam[1], Elisabeth Riegel[1], Lukas Hörmann[2], Oliver T. Hofmann[2], Oliver Gretz[1], Alfred J. Weymouth[1], and Franz J. Giessibl[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Institute of Solid State Physics, Graz University of Technology, Austria

In-plane interactions between two molecules on a surface can be used to guide on-surface chemical reactions. Our implementation to study in-plane interactions is Lateral Force Microscopy (LFM), where the tip of an AFM is oscillated laterally to directly measure the lateral forces. We investigate the short-range interactions by approaching the side of an adsorbate with a CO-terminated tip. By obtaining 3D data sets at the sides of PTCDA and CO, we demonstrated the large influence of the metal dipole at the tip apex. While previous work has noted this for strongly polarized materials, including defects in ionic crystals [1] and hBN [2], we showed that the metal tip dipole above CO must be also accounted for when measuring closer to single molecules.

1. M. Ellner et al., Nano Lett. 16, 1974 (2016). 2. F. Schulz et al., ACS Nano 12, 5274 (2018)

O 97.3 Fri 11:00 TRE Ma

Real-space imaging σ-holes and π-holes: a source of electrostatically driven non-covalent interactions — Benjamin Mallada[1,2], Martin Ondracek[1], Aurelio Gallardo[1], •Bruno de la Torre[1,2], and Pavel Jelinek[1,2] — [1]Institute of Physics, Academy of Sciences of the Czech Republic,Prague, Czech Republic. — [2]Regional Centre of Advanced Technologies and Materials, Palacký University, Olomouc, Czech Republic

Noncovalent interactions between molecules play an important role in supramolecular chemistry, molecular biology, and materials science. For the rational design/tweaking of supramolecular systems, it is helpful to understand the forces that make these systems stick to one another.

In this contribution, I will focus on the real-space visualization of the σ-hole (1) and π-hole (2). By a set of Atomic Force Microscopy (AFM), Kelvin Probe Force Microscopy (KPFM), and Scanning Tunneling Microscopy experiments we discriminate the emergence of both σ-hole and π-hole on a single molecule with unprecedented submolecular resolution. Our findings are fully supported by an atomistic model obtained from DFT calculations which allow us to simulate both AFM and KPFM images. These results may potentially open a new way to characterize biological and chemical systems in which anisotropic charges play a decisive role.

(1) B. Mallada et al. Science 2021, 374, 863 (2) B. Mallada et al. In preparation

Topical Talk O 97.4 Fri 11:15 TRE Ma

Heteroatom-substituted and three-dimensional nanocarbon materials studied with low temperature STM and qPlus AFM — •Shigeki Kawai — National Institute for Materials Science, Tsukuba, Japan

Since the first systematic on-surface covalent coupling of bromo-substituted porphyrins,[1] on-surface chemical synthesis has attracted tremendous interest of researchers. Combining with bond-resolved scanning probe microscopy (SPM) with the qPlus sensor, [2] this field has been rapidly developed. In this contribution, I will present our recent studies on on-surface chemistry with high-resolution SPM operating at low temperature under ultra-high vacuum. We synthesized heteroatom doped [3] and three-dimensional graphene nanoribbons (GNRs) by coupling bromo substituted-propellane molecules on Au(111).[4] In the 3D-GNR, the C-Br bonds distant from the surface remained intact even after the reaction. The radical species were formed by tip-induced debromination and were also stabilized by either Br atom or fullerene molecule. We also developed new on-surface reaction, which can synthesize graphene nanoribbon and covalent organic frameworks with silabenzene units by coupling Si atom and Br-substituted molecule.[5]

Reference: [1] L. Grill, et al., Nat. Nanotechnol. 2, 687. (2007). [2] L. Gross, F. Mohn, N. Moll, P. Lilkeroth, G. Meyer, Science 325, 1110 (2009). [3] S. Kawai, et al Nat. Commun. 6, 8098 (2015) and Sci. Adv. 4, eaar7181 (2018). [4] S. Kawai, et al Sci. Adv. 6, eaay8913 (2020). [5] K. Sun et al, Nat. Chem. (2022) doi:10.1038/s41557-022-01071-3.

O 97.5 Fri 11:45 TRE Ma

Interaction between an artificial and a natural atom — •Fabian Stilp, Marco Weiss, and Franz Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, Universitätsstraße 31, 93053 Regensburg

The surface state of Cu (111), a quasi-2-dimensional electron gas, is trapped to a small surface area of about 15 x 15 nm^2 by placing 48 CO-molecules in a circular shape on the surface via atomic manipulation. By doing so, one creates a quantum corral with discrete electronic states forming an artificial atom. This structure can be described reasonably well by an infinitely high circular potential well leading to corral states with Bessel-type radial functions and an angular momentum normal to the surface. To investigate the interaction between this artificial atom and a natural atom we bring Fe atoms and CO molecules inside the corral and measure the response of the corral states.

Thanks to the large corral diameter, one can study the structure of the wave functions within that artificial atom by AFM and STM showing an angular dependence of the corral states after placing the perturbations inside the corral. This change of the wave functions leads to an energy shift of a few meV. By investigating the change of the corral states due to the perturbation, one can draw conclusion about the interaction between this artificial atom and a natural atom. Here we expand the interpretation of the adatom acting repulsively on the corral states as stated by Stilp et al. [1].

[1] F. Stilp, A. Bereczuk, J. Berwanger, N. Mundigl, K. Richter, F.J. Giessibl, Science 372, 1196-1200 (2021).

O 97.6 Fri 12:00 TRE Ma

Revelation of an inhomogeneous broadening effect in artificial quantum structures caused by electron-adsorbate scattering — •Marco Weiss, Fabian Stilp, and Franz Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, Universitätsstraße 31, 93053 Regensburg

In 1993 Crommie et al. [1] arranged 48 Fe adatoms on a Cu(111) surface in a circle with a diameter of 14.26 nm. This quantum corral confines surface electrons in a circular potential well. Past investigations with scanning tunneling microscopy revealed energetically discrete eigenstates with radial Bessel functions. These studies on the Fe quantum corral showed unwanted movement of the corral walls during spectroscopic measurements because of the weak bonding of Fe on Cu(111) [1].

We used CO molecules to provide the corral with more stable walls. This permitted us to access a larger voltage window and allowed for a detailed line shape analysis of the corrals eigenenergy levels. Surprisingly, we discovered a dominant Gaussian broadening of the eigenstates.

We find that the spectral width is dependent on the size of the quantum structure. The introduction of a simple model linking the energy dependence of this inhomogeneous broadening with the single particle movement of surface state electrons has shown that the observed behaviour is compatible with an electronic lifetime limitation by interaction with the corral wall.

[1] M. F. Crommie et al., Science 262, 218-220 (1993).

O 97.7 Fri 12:15 TRE Ma

Benchmarking atomically defined probe tips for NC-AFM experiments — Damla Yesilpinar[1], Bertram Schulze Lammers[1], Alexander Timmer[1], Zhixin Hu[2], Wei Ji[3], Saeed Amirjalayer[1], Harald Fuchs[1], and •Harry Mönig[1] — [1]Westfälische Wilhelms-Universität, Münster, Germany — [2]Tianjin University, Tianjin, China — [3]Renmin University of China, Beijing, China

Controlling the identity of the tip-terminating atom or molecule in NC-AFM constitutes a milestone in surface science. We consolidate the interpretation of such studies by directly comparing the performance of four atomically defined tips: Cu-, Xe-, CO-, and O-terminated copper (CuOx-) tips. Besides their imaging performances on a metal oxide, we directly compared their capabilities in force mapping during the lateral manipulation of single adsorbed atoms. Expectedly, Cu-tips strongly react with the surface inhibiting stable imaging and picking up the atoms to be manipulated. The chemically inert Xe- and CO-tips, allow entering the repulsive force regime. However, their flexibility leads to dynamic tip bending and pronounced artefacts due to the strongly varying potential above the oxide. Furthermore, tip deflection prevents reaching sufficient threshold forces along manipulation trajectories with high energy barriers. In contrast, the combination of moderate chemical passivation and high stiffness of CuOx-tips turned out decisive for a distinct chemical-specific contrast. Moreover, this results also in a superior performance in the manipulation experiments where their high mechanical stability allows quantitative force measurements also along the trajectories with high energy barriers.

O 97.8 Fri 12:30 TRE Ma

Visualizing electrochemical interfaces with a qPlus sensor-based AFM/STM — •Andrea Auer, Bernhard Eder, and Franz Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, Germany

Atomic force microscopy (AFM) that can be simultaneously performed with scanning tunneling microscopy (STM) modes using metallic tips attached to self-sensing quartz cantilevers (qPlus sensors) has advanced the field of surface science by allowing for unprecedented high spatial resolution under ultrahigh vacuum conditions. Applying a qPlus sensor, which offers simultaneous STM/AFM and seamless transitions in between, to the field of electrochemistry creates new possibilities to locally image both the 3D layering of the interfacial water and the lateral structure of the electrochemical double layer. In this work, a home-built AFM/STM instrument equipped with a qPlus sensor for operation under precise potential control in an electrochemical liquid cell is presented. The potential-dependent structural interface organization of the electrochemical double layer on both highly oriented pyrolytic graphite (HOPG) and Au(111) electrodes in acidic media is investigated by means of (simultaneous) AFM/STM imaging and force spectroscopy. We observe frequency shift oscillations as a function of the z-piezo distance, which correspond to the layering of the interfacial solvent molecules, where both the number of layers as well as their strength is highly dependent on the applied potential.

O 98: Overview Talk Ralph Claessen

Time: Friday 13:15–14:00 Location: HSZ 03

Invited Talk O 98.1 Fri 13:15 HSZ 03

Surfaces go topological – third generation 2D quantum materials — •Ralph Claessen — Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

Metal atom-decorated semiconductor surfaces have long been studied as model systems for the formation of electrical contacts to semiconductor devices. More recently, atomic monolayers on semiconductors have come into focus as two-dimensional designer quantum materials. A case in point are two-dimensional topological insulators (2D-TIs) which host 1D metallic and spin-polarized edge states, giving rise to the quantum spin Hall (QSH) effect. Starting from the notion that a 2D honeycomb lattice favors a topologically non-trivial band structure, I will discuss several examples of such synthetic 2D-TIs, ranging from bismuthene (Bi/SiC(0001)) [1-3], whose large gap even allows the optical generation of excitons in a topological band structure [4], to indenene (In/SiC(0001)), a triangular 2D lattice of In atoms with emerging honeycomb physics and first example of a real-space obstructed QSH insulator [5, 6].

[1] Science 357, 287 (2017) [2] Nat. Phys. 16, 47 (2020) [3] Nat. Commun. 13, 3480 (2022) [4] Nat. Commun., 13, 6313 (2022) [5] Nat. Commun. 12, 5936 (2021) [6] Phys. Rev. B 106, 195143 (2022)