Surface Science Division
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

(Lecture halls H1, H3, H4, H5, H8, H9, H10, H13, H14, H15, H16, H17, H24, H25, H26 and H37, and Kunsthalle; Poster B1, B2, D, and F)

Overview Talks

O 1.1	Mon	9:30–10:15	H15	**Fundamentals of Atomic Layer Deposition** — •Stacey Bent
O 22.1	Tue	9:30–10:15	H15	**Engineered electronic states in atomic and molecular lattices** — •Peter Liljeroth
O 48.1	Wed	9:30–10:15	H15	**Catalytic activity from first principles - towards operando computational catalysis** — •Henrik Grönbeck
O 73.1	Thu	9:30–10:15	H15	**Magnetic sensing by single-atom spin resonance in an STM** — •Christopher Lutz
O 91.1	Fri	9:30–10:15	H15	**Controlling and imaging electronic structures of Quantum Materials** — •Phil King
O 100.1	Fri	13:15–14:00	H15	**From UHV to Electrochemistry - Recent Developments** — •R. Jürgen Behm

Invited and Topical Talks

O 4.1	Mon	10:30–11:00	H9	**Scaling relations and beyond for kinetic Monte Carlo models in heterogeneous catalysis** — •Mie Andersen
O 6.3	Mon	11:00–11:30	H16	**Cold water and ice: Insights from computer simulations** — •Angelos Michaelides
O 7.1	Mon	10:30–11:00	H24	**Real-time imaging of adatom-promoted graphene growth on nickel** — •Laerte L. Patera
O 8.9	Mon	12:30–13:00	H25	**Deposition and properties of ultrathin films of organic radicals** — •Maria Benedetta Casu
O 12.1	Mon	15:00–15:30	H15	**Nanoscale engineering at surfaces** — •F Stefan Tautz
O 23.1	Tue	10:30–11:00	H5	**Investigating atomic scale structure of liquid metal–electrolyte interfaces** — •Bridget M. Murphy
O 25.1	Tue	10:30–11:00	H9	**Addressing the structure and dynamics of weakly-bonded interfaces** — •Mariana Rossi
O 26.1	Tue	10:30–11:00	H15	**Imaging Electronic Correlations in Twisted Bilayer Graphene** — •Stevan Nadj-Perge
O 26.2	Tue	11:00–11:30	H15	**Designing Electronic Quantum Matter: Fabrication and Characterization with Atomic Scale Precision** — •Ingmar Swart
O 27.5	Tue	11:30–12:00	H16	**Cationic mixing in metal-supported oxide ultra-thin films: interplay of intrinsic and substrate-induced effects** — •Jacek Goniakowski, Claudine Noguera
O 32.1	Tue	14:00–14:30	H9	**The Data Revolution in Materials Science, Through the Lens of the Materials Project** — •Kristin Persson
O 36.1	Tue	14:00–14:30	H15	**Topological quantum phases in atomically precise graphene nanoribbons** — •Oliver Gröning, Shiyong Wang, Qiang Sun, Akimitsu Narita, Müllen Klaus, Pascal Ruffieux, Roman Fasel
O 36.2	Tue	14:30–15:00	H15	**Electronic properties of twisted graphene layers: bands, interactions and superconductivity.** — •Francisco Guinea

O 51.1	Wed	10:30–11:00	H9	**Theoretical Investigations of Electrochemical CO2 Reduction** — •Karen Chan
O 51.2	Wed	11:00–11:30	H9	**First-principles approach to model electrochemical reactions at the solid-liquid interface** — •Mira Todorova, Sudarsan Surendralal, Jörg Neugebauer
O 52.1	Wed	10:30–11:00	H15	**Electron-boson coupling in correlated materials: a non-equilibrium perspective** — •Claudio Giannetti, Stefano Dal Conte, Giulio Cerullo, Andrea Damascelli
O 52.5	Wed	11:45–12:15	H15	**Carrier lifetime trends in highly efficient thermoelectrics** — •Vidvuds Ozolins
O 58.1	Wed	15:00–15:30	H15	**Towards a systematic way of treating non-adiabatic effects** — •E.K.U. Gross
O 59.3	Wed	15:30–16:00	H16	**Carbon Nanomembranes: Preparation, Properties, and Applications** — •Xianghui Zhang
O 75.3	Thu	11:00–11:30	H5	**Structure evolution of oxide-supported metal nanoparticles under different conditions** — •Yuemin Wang
O 78.3	Thu	11:00–11:30	H14	**Photoemission of correlated electron pairs from metals excited by megahertz high-order harmonics** — •Cheng-Tien Chiang, Andreas Trützschler, Michael Huth, Robin Kamrla, Frank O. Schumann, Wolf Widdra
O 79.1	Thu	10:30–11:00	H15	**Enhancing quantum coherence of magnetic atoms on a surface** — •Yujeong Bae, Kai Yang, Philip Willke, Taeyoung Choi, Andreas J. Heinrich, Christopher P. Lutz
O 81.1	Thu	10:30–11:00	H24	**Zooming in on the electronic properties of van der Waals Heterostructures** — •Søren Ulstrup, Jyoti Katoch, Roland J. Koch, Simon Moser, Kathleen M. McCreary, Simranjeet Singh, Jinsong Xu, Berend T. Jonker, Roland K. Kawakami, Aaron Bostwick, Eli Rotenberg, Chris Jozwiak
O 81.2	Thu	11:00–11:30	H24	**Directly measuring the anisotropic magnetic exchange force field of a spin spiral** — •Nadine Hauptmann, Tzu-Chao Hung, Wouter Jolie, Soumyajyoti Haldar, Daniel Wegner, Stefan Heinze, Alexander A. Khajetoorians
O 81.3	Thu	11:30–12:00	H24	**Scanning Probe Microscopy at Ambient Pressures** — •Baran Eren
O 81.4	Thu	12:00–12:30	H24	**High energy surface x-ray diffraction from surfaces and particles in operando catalysis** — •Uta Hejral, Stefano Albertin, Mikhail Shipilin, Jianfeng Zhou, Sebastian Pfaff, Sara Blomberg, Johan Zetterberg, Johan Gustafson, Andreas Stierle, Edvin Lundgren
O 81.5	Thu	12:30–13:00	H24	**Batteries at Work: Towards Operando Photoelectron Spectroscopy on Lithium Ion Batteries** — •Julia Maibach, Ida Källquist, Kristina Edström, Håkan Rensmo, Hans Siegbahn, Maria Hahlin
O 83.3	Thu	15:30–16:00	H9	**Control of charge transfer into large organic molecules on ultrathin MgO(001) films** — •Martin Sterrer
O 84.1	Thu	15:00–15:30	H15	**Long-lived magnetic states in atomic-scale magnets** — •Sebastian Stepanow
O 86.5	Thu	16:00–16:30	H24	**Luttinger liquid in a box: electrons confined within MoS_2 mirror twin boundaries** — •Wouter Jolie, Clifford Murray, Philipp Weiss, Joshua Hall, Fabian Portner, Nicolae Atodiresei, Arkady Krasheninnikov, Carsten Busse, Hannu-Pekka Komsa, Achim Rosch, Thomas Michely
O 86.7	Thu	16:45–17:15	H24	**Quasiparticle interferences on Type I and Type II Weyl semimetal surfaces** — •Hao Zheng
O 96.1	Fri	10:30–11:00	H15	**Electrical transport in semiconductor nanocrystal assemblies and nanocrystal heterostructures** — •Bruno Grandidier
O 96.5	Fri	11:45–12:15	H15	**Multiprobe STM measurements of electron transport at the atomic level** — •Marek Kolmer, Wonhee Ko, An-Ping Li
O 99.1	Fri	10:30–11:00	H24	**Quantum simulation through atomic assembly** — •Sander Otte

Invited talks of the joint Symposium SKM Dissertation-Prize 2019

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:50	H2	**Synchronization and Waves in Confined Complex Active Media** — •Jan Frederik Totz
SYSD 1.2	Mon	9:50–10:10	H2	**Spin scattering of topologically protected electrons at defects** — •Philipp Rüssmann
SYSD 1.3	Mon	10:10–10:30	H2	**Beyond the molecular movie: Revealing the microscopic processes behind photo-induced phase transitions** — •Chris W. Nicholson
SYSD 1.4	Mon	10:30–10:50	H2	**Thermodynamic bounds on current fluctuations** — •Patrick Pietzonka
SYSD 1.5	Mon	10:50–11:10	H2	**Lightwave-driven quasiparticle acceleration** — •Fabian Langer
SYSD 1.6	Mon	11:10–11:30	H2	**Ultrafast plasmon-driven point-projection electron microscopy** — •Jan Vogelsang
SYSD 1.7	Mon	11:30–11:50	H2	**Helimagnets, sand patterns and fingerprints linked by topology** — •Peggy Schönherr

Invited talks of the joint Symposium Mechanically Controlled Electrical Conductivity of Oxides

See SYCO for the full program of the symposium.

SYCO 1.1	Mon	9:30–10:00	H1	**Dislocation Dynamics and Their Conductivities in Oxides** — •Yuichi Ikuhara
SYCO 1.2	Mon	10:00–10:30	H1	**Strain effects in ionic conductivity and electrode processes** — •Jürgen Janek
SYCO 1.3	Mon	10:30–11:00	H1	**Elastic dipoles of point defects in materials** — •Celine Varvenne
SYCO 1.4	Mon	11:30–12:00	H1	**Mapping strain/pressure with ZnO nanowire arrays by piezo-phototronic effect** — •Caofeng Pan
SYCO 1.5	Mon	12:00–12:30	H1	**Bulk and Flexo-photovoltaic effect** — •Marin Alexe

Invited talks of the joint Symposium Czech Republic as Guest of Honor

See SYCZ for the full program of the symposium.

SYCZ 1.1	Thu	9:30–10:00	H4	**Crystal symmetries and transport phenomena in antiferromagnets** — •Tomas Jungwirth
SYCZ 1.2	Thu	10:00–10:30	H4	**Terahertz subcycle charge and spin control** — •Rupert Huber
SYCZ 1.3	Thu	10:30–11:00	H4	**1D molecular system on surfaces** — •Pavel Jelinek
SYCZ 1.4	Thu	11:15–11:45	H4	**Tunneling microscopy on insulators provides access to out-of-equilibrium charge states** — •Jascha Repp
SYCZ 1.5	Thu	11:45–12:15	H4	**Occam's razor and complex networks from brain to climate** — •Jaroslav Hlinka
SYCZ 1.6	Thu	12:15–12:45	H4	**Long range temporal correlations in complex systems** — •Holger Kantz

Invited talks of the joint Symposium Interactions and Spin in 2D Heterostructures

See SYIS for the full program of the symposium.

SYIS 1.1	Thu	15:00–15:30	H1	**Magic Angle Graphene: a New Platform for Strongly Correlated Physics** — •Pablo Jarillo-Herrero
SYIS 1.2	Thu	15:30–16:00	H1	**Bilayer Graphene Quantum Devices** — •Klaus Ensslin
SYIS 1.3	Thu	16:00–16:30	H1	**Light-Matter interaction in van der Waals heterostructures** — •Tobias Korn
SYIS 1.4	Thu	16:45–17:15	H1	**Spin transport in Van der Waals materials and heterostructures** — •Bart Van Wees
SYIS 1.5	Thu	17:15–17:45	H1	**Flipping the valley in graphene quantum dots** — •Markus Morgenstern

Sessions

O 1.1–1.1	Mon	9:30–10:15	H15	**Overview Talk: Stacey Bent**
O 2.1–2.14	Mon	9:30–13:15	H53	**Surface Magnetism and Magnetic Coupling Phenomena (joint session MA/O/TT)**
O 3.1–3.11	Mon	10:30–13:15	H5	**New Methods and Developments I: Scanning Probe Techniques**
O 4.1–4.9	Mon	10:30–13:00	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge I (joint session O/TT/CPP/DS)**
O 5.1–5.10	Mon	10:30–13:00	H15	**Nanostructures at Surfaces I: Organics**
O 6.1–6.9	Mon	10:30–13:00	H16	**Water on Surfaces**
O 7.1–7.9	Mon	10:30–13:00	H24	**Graphene I: Structure and Growth (joint session O/TT)**
O 8.1–8.9	Mon	10:30–13:00	H25	**Metal Substrates I: Adsorption and Reactivity**
O 9.1–9.4	Mon	15:00–16:30	PHY 5.0.21	**Instrumentation Micro-/Nano-Analysis and Lithography/Structuring: Invited Talk Leo Gross (joint session KFM/DS/O)**
O 10.1–10.12	Mon	15:00–18:00	H3	**New Methods and Developments II: Scanning Probe, Spectroscopic, and Diffraction Techniques**
O 11.1–11.10	Mon	15:00–17:30	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge II (joint session O/TT/DS/CPP)**
O 12.1–12.10	Mon	15:00–17:45	H15	**Nanostructures at Surfaces II: Designer Structures and Surfaces**
O 13.1–13.10	Mon	15:00–17:30	H16	**Solid-Liquid Interfaces I: Electrocatalysis and Photoelectrochemistry**
O 14.1–14.12	Mon	15:00–18:00	H24	**Graphene II: Excitations and Nanoribbons (joint session O/TT)**
O 15.1–15.10	Mon	15:00–17:30	Kunsthalle	**Metal Substrates II: Adsorption and Reactivity**
O 16.1–16.7	Mon	15:45–18:30	H46	**Mechanically Controlled Electrical Conductivity of Oxides (joint session MM/CPP/O)**
O 17.1–17.10	Mon	17:45–20:00	Poster F	**Poster Monday: 2D Materials**
O 18.1–18.11	Mon	17:45–20:00	Poster F	**Poster Monday: Nanostructures**
O 19.1–19.10	Mon	17:45–20:00	Poster F	**Poster Monday: Organic Molecules on Inorganic Surfaces**
O 20.1–20.11	Mon	17:45–20:00	Poster F	**Poster Monday: Electronic Structure**
O 21.1–21.8	Mon	17:45–20:00	Poster F	**Poster Monday: Plasmonics and Nanooptics**
O 22.1–22.1	Tue	9:30–10:15	H15	**Overview Talk: Peter Liljeroth**
O 23.1–23.9	Tue	10:30–13:00	H5	**Solid-Liquid Interfaces II: Electrode Surfaces**
O 24.1–24.9	Tue	10:30–12:45	H8	**Plasmonics & Nanooptics I: Metastructures and Novel Techniques (joint session O/CPP)**
O 25.1–25.9	Tue	10:30–13:00	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge III (joint session O/CPP/DS/TT)**
O 26.1–26.7	Tue	10:30–12:45	H15	**Focus Session: Designer Quantum Systems I (joint session O/TT)**
O 27.1–27.9	Tue	10:30–13:00	H16	**Metal Oxide Surfaces I: Structure, Epitaxy and Growth**
O 28.1–28.10	Tue	10:30–13:00	H24	**Organic Molecules on Inorganic Substrates I: Switching and Manipulation**
O 29.1–29.10	Tue	10:30–13:00	H25	**Nanostructures at Surfaces III: Dots, Particles, and Clusters**
O 30.1–30.10	Tue	10:30–13:00	H37	**Surface Magnetism (joint session O/MA)**
O 31.1–31.10	Tue	14:00–16:30	H8	**Plasmonics & Nanooptics II: SHG and Dielectric Properties (joint session O/CPP)**
O 32.1–32.10	Tue	14:00–16:45	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge IV (joint session O/CPP/DS/TT)**
O 33.1–33.9	Tue	14:00–16:15	H10	**Solid-Liquid Interfaces III**
O 34.1–34.7	Tue	14:00–15:45	H13	**New Methods and Developments III: Spectroscopy and Tribology**
O 35.1–35.11	Tue	14:00–16:45	H14	**2D Materials I: Growth and Properties of Transition Metal Dichalcogenides, Phase Transitions**
O 36.1–36.5	Tue	14:00–15:45	H15	**Focus Session: Designer Quantum Systems II (joint session O/TT)**
O 37.1–37.11	Tue	14:00–16:45	H16	**Metal Oxide Surfaces II: Structure, Epitaxy and Growth**
O 38.1–38.11	Tue	14:00–16:45	H24	**Organic Molecules on Inorganic Substrates II: Electronic Properties and Charge Transfer**
O 39.1–39.11	Tue	18:00–20:00	Poster D	**Poster Tuesday: 2D Materials**

O 40.1–40.9	Tue	18:00–20:00	Poster D	**Poster Tuesday: Adsorption and Catalysis**
O 41.1–41.10	Tue	18:00–20:00	Poster D	**Poster Tuesday: Nanostructures**
O 42.1–42.13	Tue	18:00–20:00	Poster D	**Poster Tuesday: Organic Molecules on Inorganic Surfaces**
O 43.1–43.11	Tue	18:00–20:00	Poster D	**Poster Tuesday: Electronic Structure**
O 44.1–44.7	Tue	18:00–20:00	Poster D	**Poster Tuesday: Spins and Magnetism**
O 45.1–45.9	Tue	18:00–20:00	Poster D	**Poster Tuesday: Ultrafast Processes**
O 46.1–46.8	Tue	18:00–20:00	Poster D	**Poster Tuesday: Plasmonics and Nanooptics**
O 47.1–47.13	Tue	18:00–20:00	Poster D	**Poster Tuesday: Scanning Probe Techniques**
O 48.1–48.1	Wed	9:30–10:15	H15	**Overview Talk: Henrik Grönbeck**
O 49.1–49.8	Wed	10:30–12:30	H5	**Metal Substrates III: Structure, Epitaxy and Growth**
O 50.1–50.11	Wed	10:30–13:15	H8	**Plasmonics & Nanooptics III: STM and Time-Resolved Methods (joint session O/CPP)**
O 51.1–51.9	Wed	10:30–13:15	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge V (joint session O/CPP/DS/TT)**
O 52.1–52.7	Wed	10:30–12:45	H15	**Focus Session: Electron-Phonon Interactions I**
O 53.1–53.11	Wed	10:30–13:15	H16	**2D Materials II: Transition Metal Dichalcogenides**
O 54.1–54.10	Wed	10:30–13:00	H24	**Organic Molecules on Inorganic Substrates III: Magnetism, Doping and Interfaces**
O 55.1–55.11	Wed	15:00–17:45	H5	**Metal Oxide Surfaces III: Adsorption and Reactivity**
O 56.1–56.11	Wed	15:00–17:45	H8	**Plasmonics & Nanooptics IV: Materials Science and Chemistry Applications (joint session O/CPP)**
O 57.1–57.11	Wed	15:00–17:45	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge VI (joint session O/DS/CPP/TT)**
O 58.1–58.8	Wed	15:00–17:15	H15	**Focus Session: Electron-Phonon Interactions II**
O 59.1–59.9	Wed	15:00–17:30	H16	**2D Materials III: Nanomembranes, hBN, and Particle Interactions**
O 60.1–60.10	Wed	15:00–17:30	H24	**Organic Molecules on Inorganic Substrates IV: Electronic Properties, Excitations, Dynamics**
O 61.1–61.10	Wed	15:00–17:30	H25	**Semiconductor Surfaces: Adsorption and Reactivity**
O 62.1–62.8	Wed	17:45–20:00	Poster B1	**Poster Wednesday: Topology and Symmetry-Protected Materials**
O 63.1–63.8	Wed	17:45–20:00	Poster B1	**Poster Wednesday: Ultrafast Processes**
O 64.1–64.10	Wed	17:45–20:00	Poster B1	**Poster Wednesday: Plasmonics and Nanooptics**
O 65.1–65.16	Wed	17:45–20:00	Poster B1	**Poster Wednesday: Surface Structure, Epitaxy and Growth**
O 66.1–66.14	Wed	17:45–20:00	Poster B2	**Poster Wednesday: 2D Materials**
O 67.1–67.9	Wed	17:45–20:00	Poster B2	**Poster Wednesday: Solid-Liquid Interfaces**
O 68.1–68.11	Wed	17:45–20:00	Poster B2	**Poster Wednesday: Nanostructures**
O 69.1–69.14	Wed	17:45–20:00	Poster B2	**Poster Wednesday: Organic Molecules on Inorganic Surfaces**
O 70.1–70.10	Wed	17:45–20:00	Poster B2	**Poster Wednesday: Electronic Structure**
O 71.1–71.9	Wed	17:45–20:00	Poster B2	**Poster Wednesday: Adsorption and Catalysis**
O 72.1–72.12	Wed	17:45–20:00	Poster B2	**Poster Wednesday: Scanning Probe Techniques**
O 73.1–73.1	Thu	9:30–10:15	H15	**Overview Talk: Christopher Lutz (joint session O/MA)**
O 74.1–74.9	Thu	9:30–12:45	H32	**Focus Session: Growth, Properties and Application of Epitaxial Graphene (joint session DS/O/HL)**
O 75.1–75.9	Thu	10:30–13:00	H5	**Fundamentals of Catalysis I**
O 76.1–76.10	Thu	10:30–13:00	H8	**Plasmonics & Nanooptics V: Nanostructures and Nanoantennae**
O 77.1–77.11	Thu	10:30–13:15	H9	**Organic Molecules on Inorganic Substrates V: Solid-Liquid Interfaces, Self-Organization, Ordering**
O 78.1–78.10	Thu	10:30–13:15	H14	**Electronic Structure of Surfaces I: Photoelectron Spectroscopy**
O 79.1–79.9	Thu	10:30–13:00	H15	**Focus Session: Spins on Surfaces I (joint session O/MA)**
O 80.1–80.10	Thu	10:30–13:00	H16	**Ultrafast Electron Dynamics at Surfaces and Interfaces I**
O 81.1–81.5	Thu	10:30–13:00	H24	**Gerhard Ertl Young Investigator Award**
O 82.1–82.11	Thu	15:00–17:45	H5	**Fundamentals of Catalysis II**
O 83.1–83.9	Thu	15:00–17:30	H9	**Organic Molecules on Inorganic Substrates VI: Chirality, Charge Transfer, Self-Assembly**
O 84.1–84.11	Thu	15:00–18:00	H15	**Focus Session: Spins on Surfaces II (joint session O/MA)**
O 85.1–85.10	Thu	15:00–17:30	H16	**Ultrafast Electron Dynamics at Surfaces and Interfaces II: New Methods and Developments**

O 86.1–86.9	Thu	15:00–17:45	H24	**Topology and Symmetry-Protected Materials (joint session O/MA/TT)**
O 87.1–87.10	Thu	15:00–17:30	H25	**2D Materials IV: Charge Density Waves and Electronic Properties**
O 88.1–88.11	Thu	15:00–17:45	H26	**Electronic Structure of Surfaces II**
O 89	Thu	19:00–19:30	H1	**Annual Meeting of the Surface Science Division**
O 90	Thu	19:30–20:30	H1	**Post-Deadline Session**
O 91.1–91.1	Fri	9:30–10:15	H15	**Overview Talk: Phil King**
O 92.1–92.9	Fri	10:30–12:45	H5	**Electronic Structure Theory**
O 93.1–93.10	Fri	10:30–13:00	H8	**Plasmonics & Nanooptics VI: Near-Field Microscopy and Phenomena**
O 94.1–94.8	Fri	10:30–12:30	H9	**2D Materials V: Novel Systems**
O 95.1–95.10	Fri	10:30–13:00	H14	**Semiconductor Substrates: Metallic Nanowires**
O 96.1–96.8	Fri	10:30–13:00	H15	**Focus Session: Surface Transport at the Atomic Scale**
O 97.1–97.10	Fri	10:30–13:00	H16	**Ultrafast Electron Dynamics at Surfaces and Interfaces III**
O 98.1–98.7	Fri	10:30–12:15	H17	**Organic Molecules on Inorganic Substrates VII**
O 99.1–99.9	Fri	10:30–13:00	H24	**Focus Session: Spins on Surfaces III (joint session O/MA)**
O 100.1–100.1	Fri	13:15–14:00	H15	**Overview Talk: Jürgen Behm**

Annual General Meeting of the Surface Science Division

Thursday 19:00–19:30 H1 Audimax

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

Post-Deadline Session

Thursday 19:30–20:30 H1 Audimax

- Contributed Post-Deadline Talks

O 1: Overview Talk: Stacey Bent

Time: Monday 9:30–10:15 Location: H15

Invited Talk O 1.1 Mon 9:30 H15

Fundamentals of Atomic Layer Deposition — •Stacey Bent — Stanford University, Stanford, CA, USA

With the growing interest in functional nanoscale materials for applications such as electronics, catalysis, and energy conversion, methods for fabricating materials with atomic-level control are becoming increasingly important. Atomic layer deposition (ALD) is a vapor-based method that provides excellent capabilities for depositing thin solid films, nanoparticles, and other nanoscale inorganic materials. Based on sequential, self-limiting reactions, ALD offers exceptional conformality, thickness control at the Angstrom level, and tunable film composition. This presentation will introduce ALD and provide background on the ALD process used for growing inorganic metallic, semiconducting and insulating materials. It will also describe molecular layer deposition (MLD), in which self-limiting reactions of organic precursors lead to growth of precisely controlled, nanoscale organic thin films. Fundamental nucleation processes in ALD, including surface reactions as well as the evolution of the structure and morphology of deposited nanoscale materials, will be introduced. Moreover, many ALD nucleation processes have a dependence on the substrate upon which the film is deposited, and the ways that this property can be exploited to achieve selective deposition will also be described. Finally, the talk will showcase recent examples in which the precise control provided by ALD has been used to enable structures such as tandem solar cells and novel catalysts.

O 2: Surface Magnetism and Magnetic Coupling Phenomena (joint session MA/O/TT)

Time: Monday 9:30–13:15 Location: H53

O 2.1 Mon 9:30 H53

Magneto-Seebeck Tunneling on the Atomic Scale — Cody Friesen, •Hermann Osterhage, Johannes Friedlein, Anika Schlenhoff, Roland Wiesendanger, and Stefan Krause — Department of Physics, University of Hamburg, Germany

The tunneling of spin-polarized electrons in a magnetic tunnel junction driven by a temperature gradient is a fundamental process for the thermal control of electron spin transport. As we have shown recently, scanning Seebeck tunneling microscopy is a technique that enables spin-averaged thermopower measurements in a metal-vacuum-metal tunnel junction with atomic-scale lateral resolution [1]. Using a magnetic tip and sample allows for the experimental investigation of the details of the magneto-Seebeck tunneling, with vacuum serving as the tunneling barrier. Heating the tip with a laser and measuring the thermopower of the junction while scanning across the spin texture of the sample leads to spin-resolved Seebeck coefficients that can be determined and mapped with atomic-scale lateral resolution [2].

The experiments on Fe/W(110) and Fe/Ir(111) will be presented and discussed in terms of spin-averaged, magneto-Seebeck and anisotropic magneto-Seebeck thermopower in an ideal single atom tunnel junction. Based on the experimental findings we propose a spin detector for spintronics applications that is solely driven by waste heat, utilizing magneto-Seebeck tunneling to convert spin information into a voltage that can be used for further data processing.

[1] C. Friesen *et al.*, J. Phys. D: Appl. Phys. **51**, 324001 (2018).
[2] C. Friesen *et al.*, Science (accepted).

O 2.2 Mon 9:45 H53

Tunable spin-superconductor coupling of spin 1/2 molecules — •Luigi Malavolti[1,2,3], Matteo Briganti[4], Max Hänze[1,2,3], Giulia Serrano[4], Irene Cimatti[4], Gregory McMurtie[1,2,3], Edwige Otero[5], Philippe Ohresser[5], Federico Totti[4], Matteo Mannini[4], Roberta Sessoli[4], and Sebastian Loth[1,2,3] — [1]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany — [4]Università degli Studi di Firenze, Sesto Fiorentino (Firenze), Italy — [5]Synchrotron SOLEIL, Gif-sur-Yvette, France

Assemblies of magnetic molecules with long coherence time are being investigated as quantum bits that may be embedded in superconducting resonators [1]. Bringing the spin center into contact with the superconducting surface maximizes coupling to the resonator but may also reduce the spin's coherence time by increased scattering of quasiparticles. Here we report the capability to tune the exchange coupling of spin 1/2 vanadyl phthalocyanine molecules (VOPc) with a Pb superconducting surface. This system offers a fully tunable spin superconductor coupling from uncoupled spin to strongly coupled, screened spin [2]. These findings highlight the possibility to scale superconducting resonator experiments down to single molecule sensitivity.

[1] M. D. Jenkins, et al., Dalt. Trans. 2016, 45, 16682.
[2] L. Malavolti, et al., Nano Letters DOI: 10.1021/acs.nanolett.8b03921

O 2.3 Mon 10:00 H53

Reduced magnetic moment in polycrystalline Co thin films — •Sabine Pütter[1], Amir Syed Mohd[1], Artur Glavic[2], Stefan Mattauch[1], and Thomas Brückel[3] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ, Garching, Germany — [2]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Villigen PSI, Switzerland — [3]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) and Peter Grünberg Institute (PGI): JCNS-2, PGI-4: Quantum Materials and Collective Phenomena, Jülich, Germany

The variation of the magnetic moment with dimensionality of magnetic materials, i. e. from atoms to bulk, is a longtime studied issue. For thin films, a constant magnetic moment is often assumed in modelling, however, intermixing and surface roughness may also have an impact.

With the help of polarised neutron reflectometry (PNR) we study the magnetic moment of polycrystalline Co/20 nm Pt/MgO(001). The samples were grown by molecular beam epitaxy and subsequently measured with PNR at room temperature and in saturation in UHV.

Our results reveal the vertical depth profile of the magnetic moment of the Co films. In fact, the magnetisation is not constant but smeared out at the edges, due to roughness. Measurements at different film thicknesses reveal the evolution of the magnetic moment which is separated in a bulk and a surface contribution and discussed with respect to published results.

This project has received funding from the EU's H2020 research and innovation programme under grant agreement n. 654360.

O 2.4 Mon 10:15 H53

Investigation of the structural and magnetic properties of self-organized MnO_2 chains on Pt(001) — •Chong-Heeon Park, Martin Schmitt, Matthias Vogt, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, Würzburg, Germany

Recently, the self organized growth of 3d transition metal oxide (TMO) chains on Ir(001) and Pt(001) was investigated by STM, LEED, and DFT calculations [1,2]. Along with the structural (3×1) phase of the MnO_2 chains, antiferromagnetic (AFM) coupling on Ir(001) was predicted along and between adjacent chains. In this study, we investigate the structural and magnetic properties of self-organized MnO_2 chains, grown on Pt(001), with low temperature spin-polarized scanning tunneling microscopy (SP-STM). Similar to Ir(001), we observe a perfectly ordered $(3{\times}1)$ structural phase with an inter-chain periodicity of $3a_{\mathrm{Pt}}$. When these chains are scanned with either an in-plane or out-of-plane polarized tip (Cr-coated W tip), we observe a spin structure that can be modeled by a (15×2) magnetic unit cell. It is formed by AFM coupling along the MnO_2 chains and 72° spin spiraling across the chains.

[1] P. Ferstl, *et. al.*, Phys. Rev. B. **96**, 085407 (2017)
[2] P. Ferstl, *et. al.*, Phys. Rev. Lett. **120**, 089901 (2018)

O 2.5 Mon 10:30 H53

Coexistence of RW-AFM and 3Q state in the Mn/Re(0001) monolayer investigated with SP-STM — •Jonas Spethmann, Jonas Sassmannshausen, André Kubetzka, Roland Wiesendanger, and Kirsten von Bergmann — Institut für Nanostruktur- und Festkörperphysik, Hamburg

Exciting new physics is predicted to arise at the interface of non-collinear magnetic and superconducting materials. In order to study this subject, promising model systems need to be found. Therefore, we investigated the growth and the magnetism of a monolayer of Mn on Re(0001) using spin-polarized scanning tunneling microscopy.

Re becomes superconducting below a critical temperature of 1.69 K, which is a temperature well accessible with modern cryogenics. Mn typically prefers an antiferromagnetic order. If it is forced into a hexagonal atomic lattice, like the (0001) surface of Re, complex magnetic structures might arise due to geometric frustration. Furthermore, it is known that differently stacked monolayers of the same material can show different magnetic ground states. By adding Co to the Re surface prior to the Mn deposition, we managed to grow the Mn in two different stackings. We show that the fcc stacking exhibits a row-wise antiferromagnetic state with three symmetry-equivalent rotational domains. The hcp-stacked area shows a magnetic texture that is compatible with a so-called 3Q state [1], which is a non-collinear state with four spins in the unit cell that have an angle of 109.4° between each other.

[1] Ph. Kurz, G. Bihlmayer, K. Hirai, and S. Blügel. Phys. Rev. Lett., 86:1106-1109, Feb 2001.

O 2.6 Mon 10:45 H53

Zero field sub-10 nm skyrmions and antiskyrmions in ultrathin Co films — •Sebastian Meyer[1], Stephan von Malottki[1], Marco Perini[2], André Kubetzka[2], Roland Wiesendanger[2], Kirsten von Bergmann[2], and Stefan Heinze[1] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel — [2]Department of Physics, University of Hamburg

Non-collinear spin structures such as skyrmions are being intensively studied due to their promise for spintronic devices [1]. For applications it is envisioned to use isolated skyrmions with diameters below 10 nm that are stable at zero magnetic field [2]. Here, we use density functional theory and atomistic spin dynamics simulations [3] to show how we can stabilize magnetic skyrmions and antiskyrmions in ultrathin Co films in zero external magnetic field. In contrast to Co being a ferromagnetic material with a strong exchange stiffness we obtain very large frustration effects in the magnetic interactions of ultrathin Co films which imperatively requires an atomistic spin model. We find that the frustration enhances the energy barriers for skyrmions and antiskyrmions against collapse into the ferromagnetic ground state.

[1] A. Fert, V. Cros, and J. Sampaio, Nat. Nanotech. **8**, 152 (2013)
[2] A. Fert, N. Reyren, and V. Cros, Nat. Rev. Mater. **2**, 17031 (2017)
[3] S. Haldar, *et al.*, Phys. Rev. B **98**, 060413 (2018)

O 2.7 Mon 11:00 H53

Scanning Seebeck Tunneling Microscopy — Cody Friesen, Hermann Osterhage, Johannes Friedlein, Anika Schlenhoff, Roland Wiesendanger, and •Stefan Krause — Department of Physics, University of Hamburg, Germany

The field of spin caloritronics is specifically concerned with effects that arise in the presence of a temperature gradient, and their effect on spin-dependent electronic transport. The advent of increasingly detailed techniques for nano-scale fabrication, measurement, and manipulation have led to an improved understanding of spin caloritronic effects, and their potential uses in engineering sensors and devices at all size scales, e.g. waste-heat recycling and efficient computing.

Within this field, the thermally induced Seebeck tunneling of electrons is a fundamental effect. In our experiments, it is studied in a metal-vacuum-metal junction using scanning tunneling microscopy (STM). Selective heating of the tip with a laser generates a well-defined temperature difference at the tunnel junction. The thermovoltage between the tip and the sample is measured with atomic-scale lateral resolution and related to the band structure of the junction, as revealed by local tunneling spectroscopy. Tunnel current rectification experiments in compensated conditions allow for a direct measurement of the Seebeck coefficient without the need for tip heating, thereby realizing Seebeck mapping on the atomic scale. The STM studies will be presented and discussed in terms of thermally induced tunneling across a single-atom ideal vacuum barrier.

C. Friesen *et al.*, J. Phys. D: Appl. Phys. **51**, 324001 (2018).

15 min. break

O 2.8 Mon 11:30 H53

***Ab initio* simulations of 2D-materials interacting with magnetic clusters and surfaces** — •Nicolae Atodiresei, Vasile Caciuc, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich, Germany

Using density functional theory calculations we elucidate how the subtle interplay between the electrostatic, the weak van der Waals and the strong chemical interactions determines the geometric, electronic and magnetic structure of hybrid systems formed by magnetic substrates and atomic clusters with 2D materials as transition metal dichalcogenites (TMDs) monolayers and graphene (Gr). More precisely, the interaction between 2D and magnetic materials (i.e. surfaces, atomic clusters) shapes the (i) spin-polarization, (ii) magnetic exchange couplings, (iii) magnetic moments and (iv) their orientation of the hybrid systems. This work has been supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project number 277146847 - CRC 1238 (C01).

[1] R. Brede *et al.*, Nature Nanotech. **9**, 1018 (2014).
[2] F. Huttmann *et al.*, Phys. Rev. Lett. **115**, 236101 (2015).
[3] F. Huttmann *et al.*, Phys. Rev. B **95**, 075427 (2017).
[4] V. Caciuc *et al.*, Phys. Rev. Mat. **2**, 084001 (2018).

O 2.9 Mon 11:45 H53

Electronic and magnetic structure of monolayer and double layer GdFe/W(100) surface alloy — •Vikas Kashid, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The rare earth-transition metal alloy films are attractive materials for high density mageto-optic storage due to their magnetic recording and magneto-optical anisotropy. We investigate by virtue of spin density functional theory (DFT) as realized in the FLEUR code [1], the structural and magnetic properties of the monolayer and double layer film of GdFe on the W(100) substrate in c(2×2) unit cell, where highly localized Gd-4f orbitals are treated within GGA+U method. Gd buckles outward by 0.96 Å and 0.88 Å with respect to Fe atoms in the monolayer and double layer surfaces, respectively. The calculated monolayer and double layer GdFe/W(100) exhibits a checkerboard antiferromagnetic ground state configurations between Fe and Gd atoms. The Fe atoms in the double layer GdFe/W(100) exhibit large magnetic moment of 2.30 μ_B, larger than that of 1.45 μ_B in the monolayer film. The easy axes for the spin quantization arising from spin-orbit coupling in both the surfaces lie in the surface plane and along the diagonal of c(2×2) cell with the magneto-crystalline anisotropy energy larger for the double layer than for the monolayer.
We acknowledge discussions with Prof. Alexander Ako Khajetoorians.
[1] www.flapw.de

O 2.10 Mon 12:00 H53

Nonlocal electron correlations in an itinerant ferromagnet — •Christian Tusche[1,2], Martin Ellguth[3], Vitaliy Feyer[1], Alexander Krasyuk[3], Carsten Wiemann[1], Jürgen Henk[4], Claus M. Schneider[1,2], and Jürgen Kirschner[3,4] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-6), Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [3]Max-Planck-Institut für Mikrostrukturphysik, Halle — [4]Martin-Luther-Universität Halle-Wittenberg, Halle

A fundamental concept in solid state physics describes the electrons in a solid by the relation of the energy E vs. the crystal momentum $\boldsymbol{k}$ in a band structure of independent quasi particles. However, even for the most simple elemental ferromagnets, electron correlations are prevalent, requiring descriptions of their electronic structure beyond this simple single-electron picture. Our comprehensive measurements of the spectral-function by spin-resolved momentum microscopy show that in itinerant ferromagnets like cobalt these electron correlations are of nonlocal origin. This manifests in a complex self-energy $\Sigma_\sigma(E, \boldsymbol{k})$ that disperses as function of spin σ, energy E, and momentum $\boldsymbol{k}$. Combining the experiments with one-step photoemission calculations, we quantify the dispersion of the self-energy over the whole Brillouin zone [1]. The observation of nonlocal electron correlations in cobalt substantially affects our understanding of electron interactions, and makes itinerant ferromagnets a paradigmatic test case for the inter-

play between band structure, magnetism, and correlations.
[1] C. Tusche et al., Nat. Commun. 9, 3727 (2018)

O 2.11 Mon 12:15 H53

Magnetic coupling of ferromagnetic SrRuO$_3$ epitaxial layers separated by ultrathin spacers with large spin-orbit coupling — •Lena Wysocki[1], Michael Ziese[2], Lin Yang[1], Jörg Schöpf[1], Rolf Versteeg[1], András Kovács[3], Lei Jin[3], Felix Gunkel[4], Regina Dittmann[4], Paul H.M. van Loosdrecht[1], and Ionela Lindfors-Vrejoiu[1] — [1]University of Cologne, Institute of Physics II, Germany — [2]Felix Bloch Institute for Solid State Physics, University of Leipzig, Germany — [3]Forschungszentrum Jülich, PGI-5, Germany — [4]Forschungszentrum Jülich, PGI-7, Germany

SrRuO$_3$, a 4d ferromagnet exhibiting several Weyl nodes in proximity of the Fermi level, offers a rich playground to tailor its physical properties in epitaxial heterostructures and superlattices. Interfacing SrRuO$_3$ with large spin-orbit coupling perovskite oxides, as SrIrO$_3$, results in intriguing physical phenomena like pronounced anomalies in the Hall resistivity, attributed either to the existence of Néel type skyrmions or to modifications of the Berry curvature of electronic bands with non-trivial topology. The nature of the coupling between the magnetic layers in such superlattices is an important component influencing the global multilayer properties. We present the investigation of the magnetic coupling between ferromagnetic SrRuO$_3$ layers separated by ultrathin spacers of perovskite oxides exhibiting strong spin-orbit coupling[1]. The type and strength of the magnetic interlayer coupling was determined by major and minor magnetization measurements for various spacer geometries.
[1] L. Wysocki et al., Appl. Phys. Lett. **113**, 192402 (2018)

O 2.12 Mon 12:30 H53

Charge-transfer driven ferromagnetism in a disordered three-dimensional 3*d*-5*d* spin system — •Philipp Komissinskiy[1], Supratik Dasgupta[1], Ilya Radulov[1], Andrei Rogalev[2], Fabrice Wilhelm[2], Marton Major[1], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany — [2]European Synchrotron Radiation Facility, 71 Avenue des Martyrs, 38000 Grenoble, France

A three-dimensional disordered spin system consisting of the 3*d* transitional metal ion Mn^{4+} with strong electronic correlations and the heavy 5*d* transition metal ion Ir^{4+} with large spin-orbit coupling has been investigated in form of a perovskite thin film. The studied compound of the composition SrMn$_{0.5}$Ir$_{0.5}$O$_3$ does not exist as bulk or single crystal, but can be stabilized by epitaxy as fully disordered double perovskite thin film onto SrTiO$_3$ single-crystal substrate using pulsed laser deposition. As measured by X-ray circular dichroism, the ground state of this material is ferromagnetic with both, Mn and Ir, spins aligned in parallel. This unusual ground state can be qualitatively explained by charge-transfer driven magnetic exchange involving the effective $J = 1/2$ state of Ir. Due to the coexistence of competing magnetic interactions and randomness in the system, spin-glass features are observed at low temperatures.

O 2.13 Mon 12:45 H53

Thickness independent magnetism of the magnetic MAX phase films (Cr$_0$.5Mn$_0$.5)$_2$GaC — •Iuliia P. Novoselova[1], Andrejs Petruhins[2], Ulf Wiedwald[1], Johanna Rosen[2], Michael Farle[1], and Ruslan Salikhov[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [2]Department of Physics, Linköping University, Linköping, Sweden

Atomically laminated magnetic MAX phases M$_{n+1}$AX$_n$ (n = 1, 2, 3) have attracted interest as novel materials exhibiting both ceramic and metallic properties. Here 12.5 to 156 nm thick films (Cr$_0$.5Mn$_0$.5)$_2$GaC were investigated by ferromagnetic resonance, electron scanning microscopy and magnetometry. The X-ray diffraction reveals a high crystalline quality and phase purity. Magnetocrystalline anisotropy energy density of 140 mT as well as magnetization of 240 kA/m are found to not depend on thickness. All films are environmentally stable without a change of magnetic properties for more than one year at ambient conditions and without any protection layer. Such independence on thickness combined with the chemical stability makes the (Cr$_0$.5Mn$_0$.5)$_2$GaC films attractive for various applications such as spintronic devices or corrosion resistant magnetic sensors. This work is supported by DFG, Grant SA 3095/2-1 and DAAD Doctoral Programmes in Germany,57214224. [1] M. W. Barsoum, Prog. Solid State Chem. 28, 201 (2000).[2] A. Petruhins, et al. Journal of Mat. Sci. 50-13, 4495 (2015).[3] R. Salikhov, et al. Mat. Res, Lett. 3-3, 156-160 (2015).[4] I. P. Novoselova, Sci. Reports 8, 2637 (2018).

O 2.14 Mon 13:00 H53

The polar distortion and its relation to magnetic order in multiferroic HoMnO3 — •Nazaret Ortiz[1], Yoav William Windsor[2], Jose Renato Linares Mardegan[1], Christof Schneider[1], Gareth Nisbet[3], and Urs Staub[1] — [1]Paul Scherrer Institute, Swiss Light Source, Switzerland — [2]Fritz Haber Institut der Max Planck Gesellschaft, Germany, — [3]Diamond Light Source, United Kingdom

The orthorhombic (Pbnm) HoMnO3 is of particular interest due to its high magnetically-induced polarization values (P) and magnetoelectric coupling strength. The mechanism behind this involves high magnetic frustration, which results in a magnetic order that creates a distortion in the crystal lattice. This distortion breaks inversion symmetry and creates a macroscopic electric polarization P along the a-axis.

We investigated the atomic distortion to identify the broken symmetry of Pbnm in thin films of HoMnO3 at low temperature and the relation between the magnetic order of Ho and the structural distortion. Forbidden reflections for Pbnm has been observed, showing that the distortion does not exclusively affect to the atomic position along the polar axis, it also moves atoms along other directions. Moreover, studying reflections with component along the polar axis we observe the polar distortion directly, visualized by the difference diffraction intensity from opposite domains.

O 3: New Methods and Developments I: Scanning Probe Techniques

Time: Monday 10:30–13:15 Location: H5

O 3.1 Mon 10:30 H5

Laser Actuation of Micro Cantilevers via Thermo-Mechanical Symmetry Breaking — •Sven Kraft, Boris Hage, Ingo Barke, and Sylvia Speller — Institute of Physics, University of Rostock, 18051 Rostock

Direct actuation of Atomic Force Microscopy (AFM) cantilevers by a laser beam is particularly useful for liquid environments [1]. Various mechanisms are proposed in the literature how laser irradiation leads to mechanical cantilever excitation [2-4]. We present a systematic and comprehensive study of the spatially and frequency resolved excitation efficiency by mapping the oscillation amplitude and phase as a function of the location of an intensity modulated laser. We observe a rich mode structure with surprisingly efficient excitation at the edges, as well as multiple phase reversals in transversal direction of the cantilever, resulting in a checkerboard-like phase pattern. A comparison of coated and uncoated cantilevers, and of illumination from the top and bottom side reveals anisotropic thermal deformation being the dominant mechanism of actuation. This is corroborated by analytical calculations based on solid mechanics which take into account the cross sectional shape of the cantilevers. We also discuss the effect of an internal light intensity structure due to multiple reflection within the cantilever.

O 3.2 Mon 10:45 H5

Lateral manipulation of single iron adatoms by combined atomic force and scanning tunneling microscopy using CO-terminated tips — •Julian Berwanger, Ferdinand Huber, Fabian Stilp, and Franz J. Giessibl — University of Regensburg, 93040 Regensburg, Germany

The functionalization of scanning probe microscope (SPM) tips with a CO molecule is widely used due to their outstanding resolution capability on molecules, metal clusters and other sample systems [1-3]. However, the feasibility of CO tips for an extension of imaging by SPM to controlled atomic manipulation [4] has not been demonstrated. Here, we perform lateral manipulation of single atoms with metal and CO tips. We first study the manipulation characteristics of single atom metal tips and find that asymmetric tips, i.e. tips with a front atom that sits on a tilted atomic tip plane, yield an asymmetry in the lateral force field. When attaching a CO molecule to these tips, their asymmetric force field appears inverted with respect to the underlying tilted metal tips. By applying an analytical model, we propose that the electrostatic interaction is responsible for this inversion of the asymmetry of the lateral force field [5]. Finally we also demonstrate that CO tips can be used to reliably build up large iron clusters atom by atom starting from individual iron atoms.

[1] L. Gross et al. Science 325, 110 (2009); [2] M. Emmrich et al. Science 348, 6232 (2015); [3] M. Ellner et al. Nano Lett. 16, 3 (2016); [4] D. M. Eigler et al., Nature 344, 524 (1990); [5] J. Berwanger et al. PRB 98, 195409 (2018)

O 3.3 Mon 11:00 H5

Constant current scanning mode for imaging single molecules using low temperature atomic force microscopy with CO functionalized tips — •Daniel Martin-Jimenez[1], Doreen Mollenhauer[2], Hermann A. Wegner[3], Andre Schirmeisen[1], and Daniel Ebeling[1] — [1]Institute of Applied Physics (IAP), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Institute of Physical Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany — [3]Institute of Organic Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany

Functionalizing the tip of a low temperature atomic force microscope (AFM) with a single CO molecule facilitates imaging of single adsorbed molecules with submolecular resolution; this is often denoted as bond imaging AFM. Therewith identification of adsorption structures, reaction pathways, etc. becomes feasible. In the standard bond imaging technique, the sensor scans the samples in constant height. While this scanning mode is, in particular, suitable for types of molecules that adsorb planar to the substrate, it is incapable of imaging 3D adsorption structures. To solve this problem, we utilize a scanning mode that achieves submolecular resolution while it tracks the topography by applying a constant current. Constant height and constant current scanning modes are systematically compared and advantages and disadvantages are presented.

O 3.4 Mon 11:15 H5

Probing coherence within tunneling events in a superconducting junction — •Piotr Kot[1], Robert Drost[1], Maximilian Uhl[1], Joachim Ankerhold[2], Alfredo Levy Yeyati[3], Juan Carlos Cuevas[3], and Christian R. Ast[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Institut für Komplexe Quantensysteme and IQST, Ulm, Germany — [3]Departamento de Fisica Teorica de la Materia Condensada, Madrid, Spain

Using a superconducting tunnel junction irradiated by microwaves, we study the coherent and incoherent processes in photon-assisted tunneling. While our junction operates within the dynamical Coulomb blockade regime that involves incoherent tunneling between events, we find coherent processes within a tunneling event that can be tuned by varying the microwave intensity. We find that higher order charge transfers can not necessarily be related to the simple Tien-Gordon equation. Taking the experiment to the limit, we are able to measure coherent tunneling processes involving photons up to 50th order that do not quench superconductivity but rather distribute the spectral weight accordingly. In addition, in the high transmission regime coherence within Andreev reflections is demonstrated. Our finding suggest new avenues of studying higher order charge processes in a single junction.

O 3.5 Mon 11:30 H5

Single switching events of one molecule observed by femtosecond STM — •Dominik Peller, Thomas Buchner, Lukas Kastner, Rupert Huber, and Jascha Repp — University of Regensburg, 93040 Regensburg, Germany

Using THz waves to control electrons in a scanning tunneling microscope (STM) has opened the door to ultrafast atomic-scale microscopy. Recently, we combined low-temperature STM with ultrafast single-electron lightwave electronics to push microscopy to the ultimate spatio-temporal quantum limit via a novel state-selective tunneling regime [1]. The peak of a THz electric-field waveform transiently opens an otherwise forbidden tunneling channel through a single molecular orbital. This process allows us to record the first-ever ∼100 fs sub-Å snapshot images of a single molecule's orbitals and the first femtosecond movie of a single vibrating molecule.

Here, we introduce single-shot detection in lightwave STM as the first approach resolving individual unidirectional quantum events on simultaneous atomic and femtosecond scales. We trigger switching of an individual molecule by single-electron injection and detect every event in real time. Analyzing the quantum statistics of the different reaction paths separately, electron by electron, we time-resolve the molecule's ultrafast, statistical motion along its reaction coordinate.

Moreover, this process allows us to measure a THz near-field waveform within a subatomic volume directly in the time domain.

[1] T. L. Cocker, D. Peller *et al.*, Nature **539**, 263-267 (2016)

O 3.6 Mon 11:45 H5

Nature of binding in planar halogenbenzene assemblies and their possible visualization in scanning probe microscopy — •Aurelio Gallardo[1], Jindrich Fanfrlík[2], Pavel Hobza[2], and Pavel Jelínek[1] — [1]FZU of the CAS, Prague, Czech Republic — [2]IOCB of the CAS, Prague, Czech Republic

High-resolution scanning probe imaging of molecular structures on surfaces with functionalized tips provided the unprecedented spatial resolution. However, the origin of intermolecular features in high-resolution images of molecular assemblies is still under debate. Originally, such features were considered as a direct observation of weak non-covalent bonds between molecules. Nevertheless, this interpretation was challenged and ascribed to an experimental artefact. To address this long-standing controversy, we provided theoretical analysis of intermolecular interaction and high-resolution imaging of halogen substituted benzenes assemblies deposited on metallic substrate, which was extensively studied experimentally. First, we show that formation of molecular assemblies made of C6Br6 and C6F6 on surfaces is driven by interplay between halogen and dispersive interaction. Next, for the C6Br6 and C6F6 assemblies on surface we analyze simulated high-resolution IETS and AFM images acquired with a CO-tip. Very good agreement with the experimental evidence allows us to unambiguously determine the origin of the sharp edges. We discuss, why such sharp features should not be interpreted as the direct evidence of the signature of weak non-covalent bonds.

Gallardo et al., J. Phys. Chem. C, DOI:10.1021/acs.jpcc.8b09631

O 3.7 Mon 12:00 H5

Controlled Modulation of Plasmonic Response in a Scanning Tunneling Microscope Junction by Fabry Pérot Type Interference — •Hannes Böckmann[1], Shuyi Liu[2], Melanie Müller[2], Adnan Hammud[3], Martin Wolf[2], and Takashi Kumagai[2,4] — [1]University of Göttingen, 37077 Göttingen, Germany — [2]Department of Physical Chemistry, Fritz-Haber Institute, 14195 Berlin, Germany — [3]Department of Inorganic Chemistry, Fritz-Haber Institute, 14195 Berlin, Germany — [4]JST-PRESTO, Kawaguchi, Saitama 332-0012, Japan

We demonstrate that electroluminescence (EL) spectra from a plasmonic scanning tunneling microscope (STM) junction can be manipulated using nanofabricated Au tips by focused ion beam (FIB) milling. A broadband emission spectrum of the localized surface plasmon (LSP) resonance in the STM junction can be periodically modulated by introducing a groove structure on the FIB-polished smooth tip shaft. This groove reflects partially the propagating surface plasmon polariton (SPP) that is generated upon LSP excitation at the tip apex through inelastic electron tunneling, which consequently leads to Fabry Pérot type interference. The SPP also couples again with the LSP mode at the groove and radiates the modulated light. It is found that the emission spectra exhibit a pi phase shift between the apex and the groove, which can be rationalized by the transfer of excitation between the localized LSPs at the apex and groove through the discretized Farby Pérot like SPP levels confined in the tip shaft.

O 3.8 Mon 12:15 H5

Photon-Assisted Tunneling between Superconductors — •Maximilian Uhl, Piotr Kot, Robert Drost, and Christian R. Ast — Max-Planck-Institut für Festkörperforschung, Stuttgart

Microwaves radiated externally into a superconductor tunnel junction of a scanning tunneling microscope influence different kinds of tunneling processes. Here we use a superconducting vanadium tip and sample at a temperature of 300 mK. An external antenna has been designed to produce microwaves in a continuous range from 60 to 90 GHz [2]. It is powered through coaxial cables that are superconducting in the cooled part of the cryostat. The electric field distribution of the antenna radiation depends on the local geometry at the tunnel junction. By emitting and absorbing different numbers of photons, quasiparticles can start tunneling at energies different from the sum of the superconductors' energy gaps [1, 3]. High resolution measurements of photon-assisted tunneling in dependency of bias voltage, microwave voltage and frequency show that there is a strong transmission of the signal to the antenna. The technique of photon-assisted tunneling measurement is applied to quasiparticle as well as Cooper pair tunneling. Furthermore, it opens up new possibilities for electron spin resonance measurements.

[1] G. Falci, V. Bubanja, G. Schön: Z. Phys. B **85**, 451 (1991)
[2] J. Merkt: KIT, Bachelor thesis (2016)
[3] A. Roychowdhury et al.: Phys. Rev. Applied **4**, 034011 (2015)

O 3.9 Mon 12:30 H5

Combining high-resolution Atomic Force Microscopy with Scanning Tunneling Microscopy induced light emission on single molecules — •Katharina Kaiser, Fabian Schulz, and Leo Gross — IBM Research - Zurich, Saeumerstrasse 4, 8803 Rueschlikon

The field of STM induced light emission (STM-LE), especially on single molecules, has grown rapidly in the past 25 years [1, 2] with astounding spatial as well as energetic resolution [3, 4]. Yet, combining structural and optical information on single molecules remains challenging.

We present first results of a combined AFM and STM-LE setup on single vanadyl-phthalocyanine (VOPc) molecules. This setup so far allows for structure determination with atomic resolution by AFM with CO functionalized tips [5] and the possibility to perform controlled atom manipulation conjunct with the investigation of opto-electronic properties by STM-LE.

This work was financially supported by the European Research Council consolidator grant AMSEL.

[1] R. Berndt et al. (1993). Science, 262(5138), 1425-1427.
[2] X. Qiu et al. (2003). Science, 299(5606), 542-547.
[3] B. Doppagne et al. (2017). Phys. Rev. Lett., 118(12), 127401.
[4] A. Yu et al. (2018). Nano Lett., 18(5), 3076-3080.
[5] Gross et al. (2009). Science, 325(5944), 1110-1114.

O 3.10 Mon 12:45 H5

Near-field driven photo-assisted Scanning Tunneling Microscopy — •Benjamin Schröder[1], Ole Bunjes[1], Lara Wimmer[1], Katharina Kaiser[2], Martin Wenderoth[1], and Claus Ropers[1] — [1]Georg-August-Universität, IV. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]IBM Forschungslabor, Säumerstrasse 4, 8803 Rüschlikon

Recent developments in Scanning Tunneling Microscopy (STM) pave the way towards a controlled optical excitation of the tunnel junction with ultrafast laser pulses. This promises the local observation of surface dynamics, including photochemical reactions, phase transitions and optical manipulations of surface defects on the atomic scale.

Here, we combine an ultra-high-vacuum low-temperature STM with femtosecond laser excitation. The laser is focused directly into the tunneling junction formed by a gold tip and a Cu(100) surface. The strongly enhanced optical near field in the vacuum gap results in an additional photocurrent, evident by comparing current-distance measurements with and without laser illumination. Specifically, current-distance dependencies exhibit a contribution with a spatial decay length about ten times larger than for regular tunneling.

We employ a one-dimensional model to extract an effective energy distribution of tunneling electrons from the experimental data. We discuss contributions from multiphoton excitation and hot electron tunneling.

This project is financially supported by the DFG in the SFB 1073 (project C4).

O 3.11 Mon 13:00 H5

The steep slope to high-resolution MRFM — •Marc-Dominik Krass, Urs Grob, Raphael Pachlatko, Martin Héritier, Jan Rhensius, Alexander Eichler, and Christian Degen — Spin Physics and Imaging, ETH Zurich, Zurich, Switzerland

The goal of nanoscale magnetic resonance imaging (NanoMRI) is the 3D visualization of nuclear spin densities inside objects with near-atomic spatial resolution. One promising candidate for NanoMRI is magnetic resonance force microscopy (MRFM) which employs an ultrasensitive nanomechanical transducer to detect the interaction between nuclear spins and a magnetic field gradient [1]. In recent years, researchers have greatly improved the sensitivity of mechanical transduction [2]. At the same time, other aspects of high-resolution MRFM received little attention, even though they are just as critical.

We identify and analyze fundamental limitations of MRFM resolution and present stringent solutions to them. In particular, we shine light on the role of spin inversion pulses in the presence of thermomechanical motion, cantilever bending, and scanning stage stability. Our work should establish a recipe for subnanometer-resolution MRFM. As a result of our efforts, we demonstrate line scans with a 1D resolution below 2 nm, with a sensitivity corresponding to about 3000 protons.

[1] Christian Degen, et al., Nanoscale magnetic resonance imaging, PNAS 106, 1313 (2009). [2] William Rose, et al., High-Resolution Nanoscale Solid-State Nuclear Magnetic Resonance Spectroscopy, Phys. Rev. X 8, 011030 (2018).

O 4: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge I (joint session O/TT/CPP/DS)

First-principles electronic structure calculations have become an indispensable tool in many research areas where materials surfaces or interfaces play a central role. Corresponding calculations provide insight into catalytic mechanisms, interfacial ionic and charge transport in batteries or solar cells, materials degradation through corrosion or wear, and many other highly relevant application areas. Despite this prolific use, corresponding calculations face multiple issues. While the invited lectures will have a focus on this interface challenge, the symposium will also cover the general field of computational materials science and electronic-structure theory.

Organizers: Jens Nørskov (Technical University of Denmark), Karsten Reuter (Technical University Munich), and Matthias Scheffler (Fritz Haber Institute of the Max Planck Society, Berlin)

Time: Monday 10:30–13:00 Location: H9

Topical Talk O 4.1 Mon 10:30 H9

Scaling relations and beyond for kinetic Monte Carlo models in heterogeneous catalysis — •Mie Andersen — Theoretical Chemistry, Technische Universität München, Germany

Heterogeneous catalysis typically operates at the interface between a gas or liquid and a solid catalytic material. In my talk, I will discuss mean-field and kinetic Monte Carlo models for the operating catalyst. These often rely on input data calculated using either first principles or more approximate methods, e.g. scaling relations, which use only selected adsorption energies as descriptors for the catalyst function [1,2]. I will also discuss recent work [3] where we used compressed sensing methods to identify new low-cost and accurate descriptors that allow to predict adsorption energies for a wide range of adsorbates, multi-metallic transition metal surfaces and facets. The descriptors are expressed as non-linear functions of intrinsic properties of the clean catalyst surface, e.g. coordination numbers and d-band moments. From a single DFT calculation of these properties, we predict adsorption energies at all potential surface sites, and thereby also the most stable geometry. Compared to previous approaches such as scaling relations, we find our approach to be both more general and more accurate for the prediction of adsorption energies on alloys with mixed-metal surfaces, already when based on training data including only pure metals.

[1] M. Andersen *et al.*, Ang. Chem. Int. Ed. **55**, 5210 (2016)
[2] M. Andersen *et al.*, J. Chem. Phys. **147**, 152705 (2017)

[3] M. Andersen *et al.*, submitted

O 4.2 Mon 11:00 H9

The Teacher and the Student: Exchange-Correlation Energy Densities from Quantum Chemistry and Machine-Learning — •Johannes T. Margraf, Christian Kunkel, and Karsten Reuter — Chair for Theoretical Chemistry, Technische Universität München, Germany

(Semi-)local density functional approximations (DFAs) are the workhorse electronic structure methods in condensed matter theory and surface science. Central to defining such DFAs is the exchange-correlation energy density ϵ_{xc}, a spatial function that yields the exchange-correlation energy E_{xc} upon integration.

Unlike E_{xc}, ϵ_{xc} is not uniquely defined. Indeed, there are infinitely many functions that integrate to the correct E_{xc} for a given electron density ρ. The challenge for constructing a useful DFA is to find a systematic connection between ρ and ϵ_{xc}. While several empirical and rigorous approaches to this problem are known, there has been little innovation with respect to the fundamental functional forms of DFAs in recent years.

Herein, we discuss two less explored routes to constructing DFAs. Specifically, a recipe for deriving ϵ_{xc} directly from many-body wavefunctions is compared to a machine learning (ML) approach that infers the optimal ϵ_{xc} for a given functional form. We find that local DFAs based on the many-body ϵ_{xc} are not transferrable between systems because the underlying energy densities are inherently non-local. In contrast, the ML ϵ_{xc} is by construction as local as possible. The extension of both approaches to non-local DFAs will be discussed.

O 4.3 Mon 11:15 H9

Self-Interaction Corrected SCAN for Molecules and Solids: All-Electron Implementation with Numerical Atom-Centered Basis Functions — •Sheng Bi, Igor Ying Zhang, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Electronic self-interaction is the most severe cause of inaccuracies in all semilocal density-functional approximations (DFAs), including the promising meta-GGA "strongly constrained and appropriately normed" (SCAN) functional [1]. This error can be alleviated via localized orbital scaling corrections [2] or via self-interaction corrections (SIC) based on Fermi-orbitals [3]. In this contribution, we follow the latter concept which involves solving a set of SIC constraints. Here, we present an all-electron implementation of the self-consistent SIC for semilocal DFAs, including SCAN. We first validate our implementation by inspecting certain properties (HOMO and dissociation energies) for a molecular test set, showing that SIC improves SCAN calculations. Furthermore, we compare the performance of SCAN-SIC and SCANα, i.e., SCAN with a fraction of exact exchange, in predicting the broken symmetry in pentacene – note that standard semilocal DFAs always favor symmetric solutions. Eventually, we discuss the extension of our SIC approach to periodic solids.

[1] J. Sun *et al.*, *Phys. Rev. Lett.* **115**, 036402 (2015).
[2] N. Q. Su *et al.*, *Proc. Natl. Acad. Sci.* **115**, 9678 (2018).
[3] Z. Yan *et al.*, *Phys. Rev. A* **95**, 052505 (2017).

O 4.4 Mon 11:30 H9

Progress in Fermi-Löwdin orbital self-interaction correction to DFT — •Torsten Hahn, Sebastian Schwalbe, and Jens Kortus — Institute for Theoretical Physics, Freiberg, Germany

The accuracy of density functional theory (DFT) calculations is limited by the so called self-interaction error [1]. The recently proposed Fermi-Löwdin orbital based method [2,3,4] for self-interaction correction (FLO-SIC) is a unitary invariant and size extensive approach to overcome this error. We present the current state of the method and discuss selected applications. In addition we discuss strategies to improve the thermochemical and numerical performance of the FLO-SIC approach in combination with state-of-the-art exchange-correlation functionals.

[1] J. P. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)
[2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[3] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)
[4] S. Schwalbe et al., J. Comp. Chem., vol. 39, 2463 (2018).

O 4.5 Mon 11:45 H9

Time evolution of the natural occupation numbers — •Carlos Benavides-Riveros and Miguel A. L. Marques — Martin-Luther Universität Halle Wittenberg

Reduced density matrix functional theory (RDMFT) is based on the Gilbert theorem, which asserts that the ground-state wave function can be written as a functional of the one-body reduced density matrix. Since RDMFT accounts for fractional natural occupation numbers, it captures quite well static (strong) electron correlation (unlike DFT, RDMFT correctly predicts the insulating behavior of Mott-type insulators). Yet the time-dependent extension of RDMFT suffers from various shortcomings. Chief among them, the current status of the theory does not allow the fermionic occupation numbers to evolve in time. It is known that this deficiency is connected to the failure of RDMFT to account for relative phases at the level of the two-body reduced density matrix. Based on recent results on fermionic exchange symmetry, we propose a new equation for the time evolution of the fermionic occupation numbers.

O 4.6 Mon 12:00 H9

Nonempricial hybrid functionals constructed through adjustable potential probes for band gap predictions of extended systems — •Thomas Bischoff, Igor Reshetnyak, and Alfredo Pasquarello — Chaire de Simulation a l'Echelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

We describe a nonempirical procedure for achieving accurate band gaps of extended systems through the insertion of suitably defined potential probes. By enforcing Koopmans' condition on the resulting localized electronic states, we determine the optimal fraction of Fock exchange to be used in the adopted hybrid functional. As potential probes, we consider native defects, the extrinsic hydrogen impurity, and various adjustable potentials that allow us to vary the energy level of the localized state in the band gap and its degree of localization. By monitoring the delocalized screening charge, we achieve a measure of the hybridization with the band states, which can be used to improve the band gap estimate. Application of this methodology to AlP, C and MgO yields band gaps differing by less than 0.2 eV from experiment.

O 4.7 Mon 12:15 H9

Quantum-mechanical relation between atomic dipole polarizability and van der Waals radius — •Dmitry Fedorov, Mainak Sadhukhan, Martin Stöhr, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

The atomic dipole polarizability α and the van der Waals (vdW) radius R_{vdW} are two key quantities to describe the ubiquitous vdW forces important for the structure and dynamics of molecules and materials [1]. The commonly assumed relation between them, $R_{\mathrm{vdW}} \propto \alpha^{1/3}$, is based on a classical picture of hard-sphere atoms. Employing the quantum Drude oscillator model [2], we reveal [3] the quantum-mechanical relation $R_{\mathrm{vdW}} = const. \times \alpha^{1/7}$ which is markedly different from its classical counterpart. Based on the accessible accurate reference data for α and R_{vdW}, we demonstrate that the obtained formula can be used as a unified definition of the vdW radius solely in terms of the atomic polarizability for all chemical elements. Moreover, for vdW-bonded heteronuclear dimers consisting of atoms A and B, the simple combination rule $\alpha = (\alpha_A + \alpha_B)/2$ provides a remarkably accurate way to calculate their equilibrium interatomic distance. These findings unveil a fundamental relationship between the geometric and electronic properties of atoms. From a practical point of view, they allow us to reduce the empiricism and improve the efficiency of computational models for vdW interactions.

[1] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[2] Jones *et al.*, Phys. Rev. B **87**, 144103 (2013)
[3] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)

O 4.8 Mon 12:30 H9

impact of continuum electronic states on van der Waals dispersion interactions — •Mohammad Reza Karimpour, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

The ubiquitous van der Waals (vdW) forces play an important role for structure, stability, and dynamics of molecules and materials. Their description on atomistic level is important for molecular physics, crystal chemistry, surface science, structural biology, and pharmacy. To this end, the development of simple yet efficient models is of high importance. Normally, such models focus only on fluctuations to bound electron states, described via quantum harmonic oscillator potentials. However, the polarizability of real atomic and molecular systems has important contributions also from fluctuations to continuum states. To study their influence on the vdW dispersion interactions from a general point of view, here we consider models based on the Dirac delta-function potentials. In one-dimensional case, such a potential provides just one bound state whereas all excited states belong to the continuum electron spectrum. We apply both the atomistic method and the scattering picture representing the van der Waals and Casimir approaches for dispersion interactions, respectively. In the atomistic framework we compare our results to the ones of the quantum oscillator models. Within the other picture, we discuss an obtained new scaling law in comparison to the results known for excited atomic systems.

[1] Woods *et al.*, Rev. Mod. Phys. **88**, 045003 (2016)
[2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)

O 4.9 Mon 12:45 H9

Relation between the van der Waals radius and higher-order atomic polarizabilities — •Ornella Vaccarelli, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

The atomic polarizabilities and van der Waals (vdW) radii describe the electronic and geometric aspects of the ubiquitous vdW interactions [1, 2], respectively. Normally, these quantities are assumed to be independent. Therefore, they are determined separately from each other. Based on the quantum Drude oscillator model [3], recently we revealed [4] a remarkable direct relationship between the vdW radius and the dipole polarizability. This provides a unified determination of the vdW radius for all chemical elements solely in terms of their dipole polarizabilities. In addition, further relations between the vdW radius R_{vdW} and higher-order atomic polarizabilities α_n $(n = 1, 2, ...)$ were found empirically. Here, we present a physical background for these results. The derivation of the corresponding scaling laws is performed by going beyond the dipole approximation for the Coulomb interaction to obtain higher-order contributions to attractive and repulsive forces acting on atoms in a vdW-bonded homonuclear dimer. We focus on the derivation of the proportionality constants C_n in the general relation $R_{\mathrm{vdW}}(\alpha_n) = C_n\ \alpha_n^{2/7(n+1)}$ unveiling their quantum nature.

[1] Woods *et al.*, Rev. Mod. Phys. **88**, 045003 (2016)
[2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[3] Jones *et al.*, Phys. Rev. B **87**, 144103 (2013)
[4] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)

O 5: Nanostructures at Surfaces I: Organics

Time: Monday 10:30–13:00 Location: H15

O 5.1 Mon 10:30 H15

Ring/Chain Competition in Organometallic Oligomers with Non-Alternant Aromatic Building Blocks — •Claudio K. Krug[1], Qitang Fan[1], Damian Nieckarz[2], Florian Fillsack[1], Johannes Glowatzki[1], Nicole Trebel[1], Lukas J. Heuplick[1], Tabea Koehler[1], Paweł Szabelski[2], and J. Michael Gottfried[1] — [1]Philipps-Universität Marburg, Fachbereich Chemie, Hans-Meerwein-Str. 4, 35032 Marburg, Germany — [2]Department of Theoretical Chemistry, Maria Curie-Skłodowska University, Pl. M.C. Skłodowskiej 3, Lublin 20-031, Poland

Organometallic oligomers with C-Cu-C bonds are formed from the non-alternant aromatic compound 1,3-dibromoazulene (DBAz) after deposition on a Cu(111) surface. The oligomers appear either as macrocycles (mostly hexamers) or as chains. Depending on the DBAz coverage and the annealing temperature, the ratio between rings and chains can be tuned by kinetic and thermodynamic control. We have studied the ring/chain competition by statistical analysis of scanning tunneling microscopy (STM) images. Upon deposition at 300 K, the structure formation is kinetically controlled, resulting in the formation of mostly regio-irregular chains. Annealing theses chains to temperatures above 390 K switches the conditions to thermodynamic control, which leads to an increased yield of the thermodynamically more stable macrocycles. In the low-coverage limit, almost 80% of the deposited monomers are incorporated in cyclic hexamers. These experimental results are compared to Monte Carlo (MC) simulations, which confirm the influences of kinetic and thermodynamic control.

O 5.2 Mon 10:45 H15

Real and k-space fingerprints of a temperature driven phase transition of TPT / Cu(111) — •Lu Lyu[1], Benito Arnoldi[1], Sina Mousavion[1], Sebastian Becker[1,2], Maniraj Mahalingam[1], Benjamin Stadtmüller[1,3], and Martin Aeschlimann[1] — [1]Department of Physics, TU Kaiserslautern — [2]Department of Chemistry, TU Kaiserslautern — [3]Graduate School Materials Science in Mainz, Kaiserslautern

The design of 2D porous networks of organic molecules on metal surfaces has become a promising route to design multi-functional porous materials. Using VT-STM, LEED and Laser-ARPES, we investigate the geometric and electronic properties of monolayer 2,4,6-triphenyl-1,3,5-triazine (TPT) on Cu(111) for various sample temperatures. We find a continuously second-order phase transition in the temperature range of 297 K and 106 K, in which the TPT molecules transform from a close-packed structure to a well-ordered nanoporous-network. The mechanism can be understood by the thermodynamic competition between the intermolecular interactions (hydrogen-bonds of TPT peripheral phenyl groups) and the molecule-substrate interaction (central triazine N atoms with surface metal atoms). In the nanoporous-network phase, the standing wave of the electronic charge density can be observed in the cavities of the network in STM which coincides with the appearance of new parabolic surface states close to the Fermi level. Our findings provide a new insight into temperature-dependent electronic structures for 2D organic nanoporous-networks on noble metal surfaces.

O 5.3 Mon 11:00 H15

Molecularly resolved STM imaging of electron-induced cross-linking of aromatic self-assembled monolayers — •Patrick Stohmann[1], Sascha Koch[1], Yang Yang[1], Christopher David Kaiser[1], Niklas Biere[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, Physics of Supramolecular Systems and Surfaces, Bielefeld University, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Faculty of Physics, Experimental Biophysics and Applied Nanoscience, Bielefeld University, Universitätsstr. 25, 33615 Bielefeld, Germany

When aromatic self-assembled monolayers (SAMs) are irradiated by electrons, intermolecular cross-linking leads to the formation of carbon nanomembranes (CNMs) with molecular thickness [1], making them ideal membranes for water purification [2]. Here, we focus on the structural transformation of a pristine 4-terphenylthiol (TPT) SAM on a Au(111) surface, investigated by scanning tunneling microscopy (STM). The irradiation with electrons was carried out by employing a focused electron beam of a scanning electron microscope (SEM) at 1keV, and, for comparison, a low-energy flood gun at 50eV. The use of a combined STM/SEM microscope enables to acquire STM images before and after the irradiation steps without losing the probed sample area. We demonstrate that it is possible to study and image the initial steps of electron-induced cross-linking of the molecular layers. [1] A. Turchanin and A. Gölzhäuser, Adv. Mat. 2016, 28, 6075-6103 [2] Y. Yang et al., ACS Nano 2018, 12 (5), 4695-4701

O 5.4 Mon 11:15 H15

Coverage-dependent structural transformation of cyano-functionalized porphyrin networks on Au(111) via addition of cobalt atoms — •Brian Baker, Nico Schmidt, Mihaela Enache, and Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, Groningen, the Netherlands

The self-assembly process of a cobalt-porphyrin (Co-TCNPP) derivative containing cyanophenyl substituents at all four meso positions under ultrahigh vacuum on Au(111) was studied with room temperature scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). Deposition of Co-TCNPP onto Au(111) gave rise to the formation of a close-packed H-bonded network, which was independent of coverage as revealed by STM and LEED. A coverage dependent behavior emerged upon metal-coordination with Co-atoms. At monolayer coverage, a reticulated network exhibiting a distinct four-fold Co-coordination was formed. By reducing the molecular coverage, a structural transformation took place. The four-fold Co-coordinated network was no longer an exclusive phase and coexisted with a second metal-organic coordination network (MOCN), i.e., a chevron structure stabilized by a simultaneous expression of H-bonding and three-fold Co-coordination. We attribute the coverage-dependent structural transformation to the in-plane compression pressure exerted by the molecules deposited on the surface. Therefore, a subtle interplay between the chemical nature of the building blocks and molecular coverage can steer the formation of topologically different MOCNs and opens an alternate pathway towards the fabrication of 2D networks.

O 5.5 Mon 11:30 H15

Confined states in self-assembled $(OH)_2$-pyrene porous networks on Ag(111) — •Philipp D'Astolfo[1], Rémy Pawlak[1], Carl Drechsel[1], Thilo Glatzel[1], Silvio Decurtins[2], Shi-Xia Liu[2], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, Basel, CH 4056 — [2]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, Bern, CH 3012

Quantum dots are known to confine electrons within their structure. Recently, porous networks obtained by assembling organic molecules on metal surfaces have also shown to confine the surface electrons into their cavities, forming an array of virtual quantum dots[1-3]. Here, we investigated 2,7-Dihydroxypyrene molecules, self-assembled onto an atomically flat Ag(111) surface, using scanning tunneling microscopy (STM) and atomic force microscopy (AFM) at 4K with CO-terminated tips. Two porous network morphologies are identified that are constituted by either pure 6-member pore assemblies or mixed assemblies of 6-, 8-, and 9-member pores. By comparing their electronic properties, we found a shift of the energy levels of the confinement depending on the pore size. Interestingly, 6-member pores in the mixed assembly exhibit a +30 meV higher energy than 6-member pores in the pure counterpart, despite having the same pore diameter.

[1] Piquero-Zulaica et al., Nat. Comm., 2017, 8, 787.

[2] Lobo-Checa et al., Science, 2009, 325, 300-303.

[3] Klappenberger et al., Phys. Rev. Lett., 2011, 106, 026802.

O 5.6 Mon 11:45 H15

Self-assembled monolayers of shape-persistent macrocycles on graphite: Coadsorption with fullerene derivatives — •Joshua Bahr, Annemarie Meyer, Tristan Keller, Sigurd Höger, and Stefan-Sven Jester — Kekulé-Institut für Organische Chemie und Biochemie der Rheinischen Friedrich-Wilhelms-Universität Bonn, Bonn, Deutschland

Shape-persistent arylene-alkynylene based macrocycles form self-assembled monolayers at the solid/liquid interface of highly oriented pyrolytic graphite and 1-phenyloctane. A flexible alkoxy side chain periphery increases the solubility of the macrocyclic species in common organic solvents, and mediates its assembly into highly robust 2D networks on the solid template. In the presence of fullerenes or derivatives thereof (providing - again - increased solubility), uniform domains containing both species are formed.[1] *In situ*-STM is used to gather insights into these 2D nanoscale systems *via* submolecularly resolved images. This work focuses on understanding the interplay between the macrocycle and fullerene derivative regarding the expected binding sites. [1] G.-B. Pan, X.-H. Cheng, S. Höger, W. Freyland, *J. Am. Chem. Soc.* **2006**, *128*, 4218-4219.

O 5.7 Mon 12:00 H15

Nanopatterns of molecular squares on graphite — Kristin Gratzfeld, Nina Schönfelder, Tristan J. Keller, Sigurd Höger, and •Stefan-Sven Jester — Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Supramolecular nanopatterns of arylene-alkynylene-macrocycles at the solid/liquid interface on HOPG are studied by scanning tunneling microscopy. We recently reported on self-assembled monolayers of *molecular squares* carrying pairs of $OC_{16}H_{33}$ side chains on all four sides.[1] Here, we present a series of molecules with a reduced (*i.e.* D_{2h}) symmetry: The (still) quadratic backbones carry pairs of long and short side chains of constant ($OC_{16}H_{33}$) and variable ($OC_nH_{2n+1}, n = 6, 8, 10, 12$) chain lengths, respectively. Chains of identical lengths are observed to interdigitate intermolecularly in ABAB packing schemes. Concentration dependent polymorphism is related to robust and less robust side chain packing. The more dense polymorphs are compared with monolayers of squares that carry only $OC_{16}H_{33}$ substituents on two opposing sides. The work is part of a supramolecular surface tiling strategy. [1] S.-S. Jester, E. Sigmund, S. Höger *J. Am. Chem. Soc.* **2011**, *133*, 11062.

O 5.8 Mon 12:15 H15

Self-assembly of para-hexaphenyl-dicarbonitrile on graphene — Nico Schmidt[1], Jun Li[1], •Ida Delac Marion[1], Mihaela Enache[1], Stefano Gottardi[1], Brian Baker[1], Leonid Solianyk[1], Juan-Carlos Moreno-Lopez[1], Leticia Monjas Gomez[2], Anna Hirsch[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Groningen, the Netherlands — [2]Stratingh Institute for Chemistry, University of Groningen, Groningen, the Netherlands

We report on the self-assembly of para-hexaphenyl-dicarbonitrile (NC-Ph_6-CN) on epitaxial graphene on Cu(111) and Ir(111) as well as on highly oriented pyrolytic graphite (HOPG). Structural and electronic properties of the obtained assemblies were studied using STM, STS, and LEED. For NC-Ph_6-CN on graphene on both metallic substrates we found two related close-packed structures for which parallel molecules aligned in rows with a peculiar shift every fourth or fifth molecule, while for HOPG only one close-packed structure was observed. Hitherto the observed shift is a unique feature of NC-Ph_6-CN on graphitic substrates and already one layer of graphene is sufficient to induce it. Furthermore, we studied the formation of 1D and 2D metal-organic coordination (MOC) structures of NC-Ph6-CN and Cu atoms on graphene on Ir(111). The dimensionality of the MOC structures was tuned by varying the stoichiometry between the NC-Ph6-CN molecules and Cu atoms: for a 1:1 ratio, 1D chains based on two-fold Cu-coordination were formed, while for a 3:2 ratio, a 2D hexagonal porous network based on three-fold Cu-coordination was obtained.

O 5.9 Mon 12:30 H15

Self-assembled monolayers of molecular spoked wheels: Scanning tunneling microscopy — •Tristan J. Keller, Christopher Sterzenbach, Joshua Bahr, Taria Schneiders, Sigurd Höger, and Stefan-Sven Jester — Kekulé-Institut für Organische Chemie und Biochemie der Universität Bonn, Bonn, Deutschland

Imaging and modeling of shape persistent molecules is of great interest for 2D crystal engineering. In particular, the predictability of nanopatterns related to the molecular design and substitution pattern is a challenge. Here we report on the 2D supramolecular self-assembly of phenylene based molecular spoked wheels (MSWs). Scanning tunneling microscopy of monolayers of MSWs at the solid/liquid interfaces of highly oriented pyrolytic graphite (HOPG) and octanoic acid (OA) yields a submolecularly resolved insight into the adsorbate patterns. MSWs offer the unique opportunity to study truly shape-persistent macrocylces of well-defined geometry and symmetry. In particular MSWs with threefold rotational symmetry, and without any rotational symmetry could be investigated. Flexible alkoxy chains were used to stabilize the network formation on HOPG. The research aims at a detailed understanding of on-surface chirality of these compounds and superstructures, and more importantly on how the symmetry of the molecule influences the 2D crystal. [1] A. Idelson, C. Sterzenbach, S.-S. Jester, C. Tschierske, U. Baumeister, S. Höger, *J. Am. Chem. Soc.* **2017**, *139*, 4429-4434. [2] R. May, S.-S. Jester, S. Höger, *J. Am Chem. Soc.* **2014**, *136*, 16732-16635. [3] S.-S. Jester, V. Aggarwal, D. Kalle, *Beilstein J. Org. Chem.* **2014**, *10*, 2783-2788.

O 5.10 Mon 12:45 H15

Probing the Potential Landscape of Rotating Co(II)-5,15-diphenylporphyrin on CoO (111) Films — •Feifei Xiang and M. Alexander Schneider — Solid State Physics, Friedrich-Alexander-University Erlangen-Nürnberg, Erlangen, Germany

The adsorption of Co(II)-5,15-diphenylporphyrin (Co-DPP) on CoO (111) films of different thicknesses grown epitaxially on Ir (100) is studied by low-temperature scanning tunneling microscopy (STM) operated at 77 K. Unlike non-metalated DPP (2H-DPP), Co-DPP is observed to rotate around its metal center on CoO (111) films exceeding 1BL thickness at 77 K. By lateral manipulation, the rotation can be switched 'on' and 'off' by moving the rotating molecule to adjacent molecules. The rotating molecule appears in STM as a height modulated round feature, the modulation is attributed to the lifetime of a certain molecular orientation and reflects the local potential landscape.[1] We observe that the modulation patterns of Co-DPP vary with CoO film thickness from 2BL to 11BL. Especially the appearance of a 90° degeneracy of the potential landscape is unexpected in view of the hexagonal surface symmetry of films thicker than 2BL.

Reference

[1] Gao, L.; et al. Phys. Rev. Lett. 2008, 101 (19), 197209.

O 6: Water on Surfaces

Time: Monday 10:30–13:00 Location: H16

O 6.1 Mon 10:30 H16

Identification of OH groups from water dissociation on In_2O_3(111) with nc-AFM — •Margareta Wagner[1], Martin Setvín[1], Lynn A. Boatner[2], Michael Schmid[1], Bernd Meyer[3], and Ulrike Diebold[1] — [1]Institut für Angewandte Physik, TU Wien, Österreich — [2]Materials Science and Technology Division, ORNL, Tennessee, USA — [3]Computer Chemistry Center, FAU Erlangen-Nürnberg, Deutschland

In_2O_3 is a complex oxide material with a large unit cell where the (111) surface features a total of 12 surface oxygen atoms in four inequivalent sites. Dissociated water molecules result in two hydroxyl groups adsorbed on the surface, but only one type of surface oxygen atoms is involved in the adsorption [1]. With non-contact atomic-force microscopy (nc-AFM) we are able to identify not only the 12 individual topmost oxygen atoms of the In_2O_3(111) surface but also the individual OH groups formed upon water dissociation. Moreover, the hydrogen atom of the surface OH can be manipulated with the STM tip. This can lead to the formation of a new OH group by re-adsorption of the hydrogen atom on one of the inequivalently sited surface oxygen atoms nearby. In this work the individual OH groups are characterized and identified by their force-distance curves.

[1] M. Wagner et al., ACS Nano 11 (2017) 11531-11541.

O 6.2 Mon 10:45 H16

IR study of D_2O adsorption on K-rich feldspar — •Weijia Wang[1], Alexei Nefedov[1], Alexei Kiselev[2], Thomas Leisner[2], and Christof Woell[1] — [1]Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Institute of Meteorology and Climate Research, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

K-rich feldspar ($KAlSi_3O_8$), a widespread component of mineral dust aerosol, plays an important role in Earth's climate and the environmental sciences owing to its high efficiency in heterogeneous ice nucleation, therefore a fundamental understanding of water interaction with feldspar is necessary. Here we presented a systematic UHV infrared spectroscopy study of D_2O adsorption on K-rich feldspar substrate starting from monolayer coverages up to thick water/ice multilayers. Two specific K-rich feldspar samples were used: orthoclase and microcline. D_2O dosing on feldspar samples and IR spectra measurements were performed at low temperatures (118-150 K). IR spectra for D_2O exposing to feldspar surfaces at 118 K unraveled that amorphous solid water is formed because of the limited mobility of water molecules and the more ordered ice structures can be formed on the orthoclase surfaces compared to D_2O growth on the microcline surfaces. The structural transition of the unstable amorphous solid ice towards crystalline ice can be monitored as the sample is annealed. Dosing of D_2O on feldspar surfaces at 150 K caused ice directly into the structure of crystalline. Annealing shows the structures of the crystalline ice are thermal stable till completed water desorption occurs.

Invited Talk O 6.3 Mon 11:00 H16

Cold water and ice: Insights from computer simulations — •Angelos Michaelides — University College London, London, UK

Recent work from our research group in which we are trying to understand the intimate molecular level details of water freezing will be discussed. A particular emphasis will be placed on the role the surfaces of foreign materials play in accelerating the nucleation process [1-4] and on the dynamical nature of the nucleation event.

1. M. Fitzner, G. C. Sosso, S. J. Cox and A. Michaelides, J. Am. Chem. Soc. 137, 13658 (2015) 2. G. Sosso et al., J. Phys. Chem. Lett. 7, 2350 (2015) 3. A. Kiselev et al, Science 355, 367 (2017) 4. M. Fitzner et al., Nature Comm. 8, 2257 (2017)

O 6.4 Mon 11:30 H16

Towards Reality: Interaction of Magnetite Fe_3O_4(001) with Liquid and Ambient Pressure Water — •francesca mirabella, florian kraushofer, matthias müllner, jian xu, jiri pavelec, jan balajka, michael schmid, ulrike diebold, and gareth parkinson — Technische Universität Wien, Vienna, Austria

Water interaction with iron oxides plays an important role in different fields. The structure of the solid-liquid interface often defines the performance of a material in its applications. As a first step, we studied the stability of a UHV-prepared Fe3O4(001)-($\sqrt{2} \times \sqrt{2}$)R45° surface upon interaction with water vapor as well as liquid. We used a new experimental setup that allows to bring a UHV-prepared surface in direct contact with ultrapure liquid water (and vapor) without exposure to air. The effect of water on the surface was then studied with low energy electron diffraction (LEED), X-ray photoemission spectroscopy (XPS) and scanning tunneling microscopy (STM). XPS data show that the surface is hydroxylated upon short exposure (seconds) to ultra-pure liquid H2O. After longer exposure (minutes-hour), STM shows new features, namely rows growing on top of the pristine surface. The growth of these rows is accompanied by a stronger hydroxylation of the surface (XPS) and lifting of the ($\sqrt{2} \times \sqrt{2}$)R45° reconstruction (LEED). XPS data, several control experiments, and reproducibility in two different UHV chambers let us exclude any contamination. The formation of these rows seems to be restricted to the surface layer. We interpret them as iron-(oxy)-hydroxide species formed by excess iron diffusing out from subsurface layers in a kinetically-limited process.

O 6.5 Mon 11:45 H16

Nickel doping enhances the reactivity of Fe_3O_4(001) to water — •Zdenek Jakub, Jan Hulva, Francesca Mirabella, Florian Kraushofer, Matthias Müllner, Michael Schmid, Ulrike Diebold, and Gareth S. Parkinson — Institute of Applied Physics, TU Wien, Austria

Spinel ferrites are technologically important materials showing high catalytic activity for oxygen evolution and water gas shift reactions. In our previous work we've described water adsorption on Fe_3O_4(001), which is also a well-documented model surface for single-atom reactivity studies. In this work we focus on the water adsorption on nickel-enriched Fe_3O_4(001) surface. Using scanning tunneling microscopy, temperature programmed desorption and x-ray phototemission spectroscopy we show nickel adatoms activate the surface for water dissociation and adsorption above room temperature. At the same time, the presence of nickel adatoms on the surface blocks the formation of partially-dissociated water dimers and trimers which are observed on the clean surface. Interestingly, this result does not change when the adatoms get incorporated into the surface by thermal annealing.

O 6.6 Mon 12:00 H16

Understanding an electrochemical interface from first principles: the case of hematite. — •Nicola Seriani — The Abdus Salam ICTP, Trieste, Italy

In photocatalytic water splitting, crucial processes take place at the interface between the photocatalyst and the liquid electrolyte, and are influenced by the structure of the interface itself. We have investigated the electrical double layer at the interface between hematite and water at different values of pH, by means of ab-initio simulations based on density functional theory. We show how charging of the surface determines the structure and dielectric properties of the interface, and the interaction of hematite with water. These results help the interpretation of electrochemical measurements, and provide new insight into the kinetics of the water splitting reaction.

O 6.7 Mon 12:15 H16

Visualizing the atomic edge structure of a two-dimensional ice with atomic force microscopy — •Runze Ma[1], Duanyun Cao[1], Chongqin Zhu[2], Ye Tian[1], Xiaocheng Zeng[2], Limei Xu[1,3], Enge Wang[1,3], and Ying Jiang[1,3] — [1]International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, P. R. China — [2]Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588, United States — [3]Collaborative Innovation Center of Quantum Matter, Beijing 100871, P. R. China

Low-dimensional water is responsible for a broad spectrum of phenomena in materials science, nanoscience, chemistry, biology, and geology. Especially, the edges of ice play key roles in the ice growth/melting, catalytic reaction and molecular adsorption, but atomic-scale structural characterization still remains a big challenge so far due to the fragileness and high reactivity of the ice edges.

Here we report atomic-scale imaging of the edge structures of a two-dimensional bilayer ice grown on Au(111) surface with non-contact atomic force microscopy. We found that the armchair edges coexist with the zigzag ones, with almost comparable population. We were able to deduce different growth behaviors for the zigzag and armchair edges from the frozen metastable or intermediate structures at the two edges.

This work not only reveals new understanding of the stability and growth of two-dimensional ices, but also opens up new possibility of probing structure and dynamics of "ice at the edge" in real space.

O 6.8 Mon 12:30 H16

Local Signature of Solvated Electrons — •Cord Bertram[1,2], Philipp Auburger[3], Michel Bockstedte[3,4], Julia Stähler[5,6], Uwe Bovensiepen[2,6], and Karina Morgenstern[1] — [1]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum — [2]Fakultät für Physik, Universität Duisburg-Essen — [3]Lehrstuhl für Theoretische Festkörperphysik, Friedrich-Alexander Universität Erlangen-Nürnberg — [4]Chemie und Physik der Materialien, Universität Salzburg — [5]Physikalische Chemie, Fritz-Haber-Institut der Max-Planck-Gesellschaft — [6]Fakultät für Physik, Freie Universität Berlin

Electron solvation, like any solvation, induces transient molecular rearrangements of the solvent molecules, which are important for understanding fundamental processes in various scientific fields like surface science and electrochemistry. We investigated the impact of electron solvation on the local, molecular structure at ice surfaces on Cu(111) with low temperature scanning tunneling microscopy, two-photon photoemission, and ab initio theory. UV photons generate excited electrons in Cu(111), which penetrate the conduction band of the ice and solvate at its surface. The electron solvation leads not only to a transient reorientation of water molecules on ice surfaces, but also to permanent structural changes and the motion of individual molecules. These changes occur predominantly close to defect sites because of the defect's abundance of polar dangling OH groups. Our results suggest that fast energy dissipation during solvation triggers permanent molecular rearrangement via vibrational excitation. This work is supported by the DFG through the cluster of Excellence RESOLV (EXC 2033).

O 6.9 Mon 12:45 H16

Single ion hydrates under the SPM tip — •Jinbo Peng[1], Duanyun Cao[1], Zhili He[1], Jing Guo[1], Prokop Hapala[2], Runze Ma[1], Bowei Cheng[1], Ji Chen[3], Wen Jun Xie[1], Xin-Zheng Li[1], Pavel Jelínek[2], Li-Mei Xu[1], Yi Qin Gao[1], En-Ge Wang[1], and Ying Jiang[1] — [1]Peking University — [2]Czech Academy of Sciences — [3]University College London

Ion hydration and transport at interfaces are relevant to a wide range of applied fields and natural processes. To correlate atomic structure with the transport properties of hydrated ions, both the interfacial inhomogeneity and the complex competing interactions among ions, water and surfaces require detailed molecular-level characterization. Here we constructed individual sodium ion (Na+) hydrates on a NaCl(001) surface by progressively attaching single water molecules to the Na+ using a combined scanning tunnelling microscopy(STM) and atomic force microscopy(AFM) system. We found that the Na+ hydrated with three water molecules diffuses orders of magnitude more quickly than other ion hydrates. Ab initio calculations revealed that such high ion mobility arises from the existence of a metastable state, in which the three water molecules around the Na+ can rotate collectively with a rather small energy barrier. Our work suggests that anomalously high diffusion rates for specific hydration numbers of ions are generally determined by the degree of symmetry match between the hydrates and the surface lattice. Reference: Peng, J. et al. Nature 557, 701 (2018) Peng, J. et al, Nat. Commun. 9, 122 (2018)

O 7: Graphene I: Structure and Growth (joint session O/TT)

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

Invited Talk O 7.1 Mon 10:30 H24

Real-time imaging of adatom-promoted graphene growth on nickel — •Laerte L. Patera — Department of Physics, University of Trieste, 34127 Trieste, Italy — IOM-CNR - TASC Laboratory, Basovizza, 34149 Trieste, Italy — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Single adatoms are expected to participate in many processes and chemical reactions occurring at solid surfaces. We demonstrate, both experimentally and theoretically, the catalytic role played by single metal adatoms during the graphene growth on Ni(111). The catalytic action of individual Ni atoms at the edges of a growing graphene flake was directly captured by scanning tunneling microscopy imaging at video-rate, allowing the precise determination of the atomic structure of reaction intermediates in the ms time-scale. Force field molecular dynamics and density functional theory calculations rationalize the experimental observations. Our results unveil the mechanism governing the activity of a single-atom catalyst at work [1].

[1] L. L. Patera et al., Science 359, 1243-1246 (2018)

O 7.2 Mon 11:00 H24

Adsorption Heights and Coupling Strength at Graphene/Ni(111) and h-BN/Ni(111) interfaces — •Christina Schott[1], Johannes Seidel[1], Markus Franke[2], Anja Haags[2], You-Ron Lin[2], Martin Aeschlimann[1], Christian Kumpf[2], and Benjamin Stadtmüller[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Peter Grünberg Institut, Functional Nanostructures at Surfaces, 52425 Jülich, Germany

From a technological point of view, 2D material stacks consisting of light elements grown on ferromagnetic surfaces are highly promising for spintronic applications due to their low spin-orbit coupling and the large charge and spin carrier velocity. However, utilizing the exotic properties requires a minimization of the chemical interaction between the 2D layers and the ferromagnet. Therefore, we have investigated the interlayer interaction strength and coupling mechanisms in bilayer films of prototypical 2D materials on the ferromagnetic surface Ni(111) by using the NIXSW technique. The small vertical bonding distance between graphene or the nano-graphene molecule coronene and the Ni(111) surface suggests a strong chemical interaction across the interface. To achieve a decoupling of coronene from Ni, we used one layer of h-BN as a buffer layer between one the coronene layer and the Ni substrate. Here, we will discuss the modifications of the vertical adsorption height of gr and coronene upon the passivation of the Ni surface and correlate our findings to the chemical interaction and the vertical distortions of these 2D layers.

O 7.3 Mon 11:15 H24

Thermodynamically Stable Small-Angle Twisted Domains in Graphene on Iridium (111) — •Karim M. Omambac[1], Christian Brand[1], Hichem Hattab[1], Laurenz Kremeyer[1], Giriraj Jnawali[1], Alpha T. N'Diaye[2], Johann Coraux[2], Raoul van Gastel[3], Bene Poelsema[3], Thomas Michely[2], Frank-Jörg Meyer zu Heringdorf[1], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen, Germany — [2]Universität zu Köln, Germany — [3]University of Twente, The Netherlands

Lattice rotations or twists is one to the characteristics in the catalytic growth of monolayer graphene on a hot metallic surface. In particular, these small-angle twists have not yet been found experimentally but have been predicted partly through density functional theory calculations [1]. In this low energy electron diffraction study we evaluated the distribution of twisted domains of the epitaxially grown graphene on Ir(111) through spot profile analysis of the moiré spots. We find a new class of small-angle twisted domains with clear and distinct twist angles of 1.7°, 1.1° and 0.6° at growth temperatures of 1255 K, 1350 K, and 1460 K, respectively. To further analyze, we performed a simple two-dimensional in-plane coincidence site lattice analysis taking only into account the thermal expansion coefficients between the substrate and the epitaxially grown graphene. The results show a very good agreement with the experimental findings suggesting the origin of these small-angle twisted domains is strongly dependent on the variation of the lattice mismatch between graphene and Ir(111) substrate during growth. [1] J. Phys.: Condens. Matter **24**, 314214 (2012)

O 7.4 Mon 11:30 H24

Buckling of graphene on Ir(111) by the intercalation of cobalt — •David A Duncan[1], Nicolae Atodiresei[2], Simone Lisi[3], Phil J Blowey[1,4], Vasile Caciuc[2], James Lawrence[4], Tien-Lin Lee[1], Maria Grazia Betti[5], Pardeep Thakur Kumar[1], Ada Della Pia[5], Giovanni Costantini[4], and D. Phil Woodruff[4] —

[1]Diamond Light Source, Didcot, UK — [2]Forschungzentrum Jülich, Jülich, Germany — [3]Institut Néel, Grenoble, France — [4]University of Warwick, Coventry, UK — [5]University Sapienza of Rome, Rome, Italy

The intercalation of Co between graphene and Ir(111) results in a corrugated network of strongly and weakly bound carbon [1]. Utilising the X-ray standing wave method to monitor the chemical-state resolved C 1s photoemission components [2], we determine that the strongly bound C atoms adsorb with a mean adsorption height, above the Co layer, of 2.06(3) Å, almost 0.75 Å lower than that of the weakly bound C atoms (2.76(5) Å). DFT calculations using DFT-D2 and vdW-DF corrections predict a subtle difference corrugation structure, with DFT-D2 predicting a local maximum where the vdW-DF predicts a global minimum. The DFT-D2 calculations result in a structural model that more closely matches the experimental results, with the vdW-DF calculations predicting mean adsorption heights for the strongly and weakly bound C atoms that are 0.10 Å and 0.37 Å closer to the Co intercalant, respectively, than measured experimentally. Despite this difference, both functionals predict a covalent like interaction between the Co and the C, resulting in a weak nearest-neighbour C-C buckling.

[1] PRB 87 (2013), 041403; [2] PRB, 90 (2014), 195446

O 7.5 Mon 11:45 H24

Understanding the first steps of graphene growth: a study of small carbon clusters on Cu surfaces — •Juan Santiago Cingolani, Mie Andersen, and Karsten Reuter — Chair of Theoretical Chemistry, Technical University of Munich, Germany

It has been shown that high quality single layer graphene can be obtained through chemical vapor deposition on liquid Cu [1]. The role of the liquid surface in carbon nucleation as well as in defect healing is not yet well understood. While a comprehensive description of the growth mechanism would require molecular dynamics (MD) simulations, a first step is to study the precursors for graphene growth and the influence of the surface on them.

We performed a series of density-functional theory (DFT) calculations of carbon clusters of different sizes adsorbed to different Cu facets aiming to shed some light on the effects of the surface on relative stabilities, as well as on experimentally accessible properties such as vibrational frequencies. We also take advantage of the data generated to fit the parameters of density-functional tight binding, a semi-empirical method, which in turn allows us to carry out MD simulations for longer timescales and in larger systems than otherwise accessible through *ab initio* methods. We then simulate graphene flakes on liquid Cu at different levels of theory to get a clearer picture of what the Cu surface might look like under growth conditions.

[1] L. Tan, M. Zeng, T. Zhang, L. Fu, Nanoscale 7, 9105 (2015).

O 7.6 Mon 12:00 H24

Aperiodically ordered nano-graphene — •Mahalingam Maniraj[1], Lu Lyu[1], Sebastian Becker[1,2], Dominik Jungkenn[1], Sebastian Emmerich[1], Sina Mousavion[1], D L Schlagel[3], T A Lograsso[3], Sudipta Roy Barman[4], Stefan Mathias[5], Benjamin Stadtmuller[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany — [2]Department of Chemistry, TU Kaiserslautern, Germany — [3]Division of Materials Sciences and Engineering, Ames Laboratory, USA — [4]UGC-DAE Consortium for Scientific Research, Indore (M.P.), India — [5]I. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

We demonstrate that the quasiperiodic order of surfaces can be transferred to 2D adsorbate systems by investigating the self-assembly of the nano graphene molecule coronene on the icosahedral(i)-Al-Pd-Mn quasicrystalline surfaces using multiple surface sensitive techniques. We find a quasiperiodic ordering of coronene on the i-Al-Pd-Mn surface which can be explained qualitatively by the P1 Penrose tilling. Using angle resolved photoemission spectroscopy, we observe a 5-fold symmetric modulation of the photoemission intensity distribution in the kx-ky-plane with a clear band dispersion along the high symmetry axis in momentum space. The latter suggests a direct correlation between the energy and momenta of the electrons in the quasicrystal and the rotational symmetry of the system. Moreover, the pseudogap of the bare Al-Pd-Mn persists even after the adsorption of the aperiodically ordered coronene confirming the quasiperiodic nature of the interface.

O 7.7 Mon 12:15 H24

The role of the curvature of graphitic materials in the oxygen adoption reaction — Jakob Hauns, Julian Wüst, Jürgen Weippert, Regina Fischer, Frank Hennrich, Dmitry Strelnikov, •Artur Böttcher, and Manfred M. Kappes — Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

The capability of graphitic materials to bind atomic oxygen has been studied under ultrahigh vacuum conditions by monitoring the oxygen-induced evolution of the XPS-*O1s*, -*C1s* and the valence band states, UPS-VB. Three groups of solid films were investigated: HOPG (planar graphene sheet), felts of metallicity-sorted single walled carbon nanotubes S-, M-SWCNTs and solid C_{60} films. The monodispersed materials chosen here differ by the curvature ***C*** of the graphene layers. In order to quantify the role of strained C-C-C bonds in the oxidation pathway exactly the same oxidation procedure has been applied to all graphitic materials. The VB-DOS profiles measured for oxidized films differ clearly by their oxygen-derived bands and the work functions. The evolution of the XPS-*O1s* and -*C1s* states indicate that whereas the oxidation of planar graphene sheets proceeds via epoxy species [1], ether functionalities dominate the oxidative scenario of the curved surfaces of SWCNT and **C$_{60}$**. The yield for the initial oxygen-adoption reaction for all curved surfaces is significantly higher than that measured for planar graphene sheets. This finding stresses the unique role of the strained -C-C-C- bonds which facilitate the formation of ether functionalities. [1] A. Barinov, et al. J. Phys. Chem. C 2009, 113, 9009.

O 7.8 Mon 12:30 H24

Thermal reduction of graphene oxide studied by electron spectroscopy — •Gianluca Di Filippo[1], Andrea Liscio[2], and Alessandro Ruocco[1] — [1]Dipartimento di Scienze, Università degli Studi Roma Tre, Rome, Italy — [2]Consiglio Nazionale delle Ricerche, Istituto per la Microelettronica e Microsistemi, Rome, Italy

Graphene oxide (GO) is a purely 2D material composed of a conductive filter given by sp^2 domains and an insulating matrix containing sp3-carbons, defects, holes and oxygen functional groups. The latter make GO an insulator, but its electronic, optical and structural properties can be tailored via controlled removal of the oxygen groups. This enables reduced graphene oxide (rGO) to be used in many fields such as sensors development and energy storage applications.

In this work, we investigated the thermal reduction of GO in ultra-high-vacuum by combining several electron spectroscopies. Photoemission spectroscopy (XPS and UPS) was used to investigate variations in the chemical and electronic structure of GO reduced in the 150 °C - 750 °C temperature range. The optical properties of rGO were investigated using electron energy loss spectroscopy (EELS). The build-up of the $\pi-$plasmon excitation was observed upon reduction at 300 °C, this revealing the formation of ordered graphene-like areas with dimensions around 5 nm. The vibrational spectrum revealed the presence of CH groups on the surface. Most of the hydrogen atoms are bound to sp^3-carbon and are probably located in oxidized regions in the basal plane of rGO. The sp^3-CH impurities can be removed upon annealing at 750 °C where only sp^2 CH defects are observed.

O 7.9 Mon 12:45 H24

Intercalation dynamics of sulfur underneath graphene on Ru(0001) — •Lars Buss[1], Jens Falta[1,2], and Jan Ingo Flege[3] — [1]Institute for Solid State Physics, University of Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Germany — [3]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany

It is known that the binding of epitaxially grown graphene to the substrate has a detrimental effect on its electronic properties. This is especially true for the strong binding to various transition metals and particularly ruthenium. However, via intercalation the interlayer coupling can be lifted and its unique electronic properties can be restored. Therefore, we have investigated the interaction of sulfur with single-layer graphene grown on Ru(0001) via surface segregation and CVD of ethylene under UHV conditions with in situ low-energy electron microscopy (LEEM) and micro-diffraction (μLEED). At elevated temperature and under dimethyl disulfide background pressure, we observe that sulfur intercalates through the open edges of the graphene islands. Prolonged exposure to sulfur induces wrinkling of the graphene islands, consistent with substantial relief of tensile strain after successful sulfur insertion underneath the graphene. It can be seen that the intercalation dynamics are both dependent on the temperature during intercalation and the preparation method of the graphene sheets. Furthermore, darkfield imaging and μLEED of the intercalated graphene reveal a graphene induced improved ordering of sulfur underneath.

O 8: Metal Substrates I: Adsorption and Reactivity

Time: Monday 10:30–13:00 Location: H25

O 8.1 Mon 10:30 H25

Interaction of AuZn surfaces with oxygen species and formation of ZnO_x on Au(111) — •Konstantin M. Schüttler, Albert K. Engstfeld, Joachim Bansmann, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Au/ZnO is a highly active catalyst for the synthesis of "Green Methanol" from CO_2 and H_2, where the latter should stem from renewable sources [1]. Industrially, Cu/ZnO is used for MeOH synthesis, where under reaction conditions ZnO at the perimeter of the Cu nanoparticles is partly reduced, forming bimetallic CuZn sites [2]. For Au/ZnO catalysts, AuZn formation would be similarly plausible.

In order to gain more insight into the formation, structural, electronic and chemical properties of AuZn sites, bimetallic Zn/Au(111) model catalyst surfaces were studied under UHV conditions. We investigated the interaction of Zn surface atoms with oxygen by exposing various AuZn nanostructures to molecular and atomic oxygen. Furthermore we illustrate the thermal stability of the newly formed nanostructures. Second, we explored the formation of ZnO_x/Au(111) $(0 \leq x \leq 1)$ and studied the species formed depending on the oxidation conditions. Consequences of these findings on our understanding of realistic Au/ZnO catalysts are discussed.

[1] Y. Hartadi et al., ChemSusChem 8 (2015), 456
[2] S. Kuld et al., Angew. Chem. Int. Ed. 53 (2014), 5941

O 8.2 Mon 10:45 H25

Ground state structure for 0.5 ML oxygen on Rh(100) — Tilman Kisslinger[1], Margareta Wagner[2], Michael Schmid[2], Ulrike Diebold[2], •M. Alexander Schneider[1], and Lutz Hammer[1] — [1]Ls. f. Festkörperphysik, Univ. Erlangen — [2]Inst. f. Angewandte Physik, TU Wien

The structure of 0.5 ML oxygen on Rh(100) was so far reported by experiment [1] and theory [2] to be a (2×2)-2O supercell where O sits on threefold hollow sites of the clockwise-anticlockwise reconstructed Rh(100). Newly taken LEED-IV data at first sight confirm this model with a quite low Pendry R-factor of R = 0.12. However, like in [1] the model fails to explain extinctions of diffraction spots in the LEED pattern and it also disagrees with DFT calculations that predict a 12 pm buckling between surface Rh atoms. Allowing for positional disorder of oxygen within the (2×2)-2O cell improves the fit of our LEED-IV data taken at 100 K and restores the symmetry elements. By STM at room temperature a (2×2) periodicity is found while at 77 K and 4 K the system is well-ordered with c(4×4)-4O surface cell. Applying DFT to a model with alternate occupation of threefold hollow sites by oxygen atoms reproduces the experimental STM image and shows that the c(4×4)-4O is energetically more favourable than the (2×2)-2O by 4 meV per oxygen atom. Furthermore, the new model describes the LEED-IV data with R = 0.08 even better, i.e. the structural elements of the c(4×4)-4O are locally present also at 100 K. [1] A. Baraldi et al., PRL **82**, 4874 (1999) [2] D. Alfè et al., Surf. Sci. **410**, 151 (1998)

O 8.3 Mon 11:00 H25

Oxidation of Transition-Metal Surfaces at Realistic Temperature and Pressure Conditions — •Zhong-Kang Han[1], Ray Miyazaki[2], Somayeh Faraji[1], Santiago Rigamoni[3], Maria Troppenz[3], Claudia Draxl[3,1], Jun-ya Hasegawa[2], Sergey V. Levchenko[4,1,5], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Hokkaido University, Sapporo, JP — [3]Humboldt–Universität zu Berlin, Berlin, DE — [4]Skolkovo Innovation Center, Moscow, RU — [5]NUST MISIS, Moscow, RU

Oxidation of metal surfaces is a ubiquitous phenomenon, but its thermodynamics is still not fully understood. Using the all-electron FHI-aims code, we perform a systematic DFT study (comparing various xc approximations) for the adsorption of atomic oxygen at (111) and (110) surfaces of Au, Pt, Ni, Pd and Cu, and the Pd- or Pt-alloyed Cu(111) and (110) surfaces. The finite-temperature thermodynamics is evaluated using a cluster expansion. At low coverages (<25%) O atoms are predicted to adsorb randomly at the short-bridge sites of elemental metal (110) surfaces, and they form a $c(2 \times 2)$ pattern when the coverage increases, until a new $c(2 \times \sqrt{2})$ pattern forms with top and hollow sites occupied. Quite differently, at (111) surfaces a variety of ordered adsorbed O phases is found, with a mixed occupation of the fcc and hcp hollow sites. The structures of adsorbed O at the alloyed surfaces exhibit a larger variety of patterns depending on coverage, with Pd/Pt segregating to the surface at low O chemical potentials (i.e., higher temperatures and/or lower O_2 pressures), while increasing the chemical potential induces Cu segregation.

O 8.4 Mon 11:15 H25

Modeling the formation and reactivity of surface oxide islands on metal surfaces — •Albert Bruix and Karsten Reuter — Technical University of Munich (Germany)

The surfaces of many transition metals are oxidized under ambient conditions or at increased oxygen pressures, which has strong implications for corrosion and catalysis. Stable O-enriched states resulting from oxidation may consist of the metal surface with high concentration of adsorbed O atoms, the corresponding metal-oxide, or something in between. The latter include surface oxides, i.e. ultrathin oxide layers formed on the surface of the metal.

A quantitative atomistic modeling of oxidation reactions catalyzed on such transition metals therefore requires an understanding of the chemical properties and formation mechanisms of the oxidized surfaces. In this work, PdO(101) surface oxide islands on the Pd(100) surface are studied by means of Density-Functional Theory calculations. We first establish a thermodynamic model for the formation and growth of surface oxide islands, focusing on the stability of different island edge types. We then use a multi-lattice microkinetic modeling approach to investigate the role of the metal and surface oxide phases, and how their coexistence under different operation conditions affects catalytic performance. Our approach also allows probing the relevance of sites at the interface between the two phases and the effect of phase transitions on the overall reactivity.

O 8.5 Mon 11:30 H25

The effect of temperature in plasmon driven reactions — •Wouter Koopman[1], Radwan Sarhan[1,2], Ferenc Liebig[3], Jan Pudell[1], Marc Herog[1], Matthias Rössle[4], Thomas Schmid[2,5], Sebastian Schmitt[4], Felix Stete[1,2], Clemens Schmitt[6], Joachim Koetz[3], and Matias Bargheer[1,4] — [1]Institute of Physics and Astronomy, University of Potsdam — [2]School of Analytical Sciences Adlershof, Humboldt-Universität zu Berlin — [3]Institute of Chemistry, University of Potsdam — [4]Helmholtz Zentrum Berlin — [5]Federal Institute for Materials Research and Testing, Berlin — [6]Max Planck Institute of Colloids and Interfaces, Potsdam

Metal nanoparticles form potent nanoreactors, driven by the optical generation of energetic electrons and nanoscale heat. The relative influence of these two factors on nanoscale chemistry is strongly debated. We investigate the temperature dependence of the dimerization of 4-NTP into DMAB adsorbed on goldnanoflowers.Static X-ray diffraction and Raman thermometry indicate a temperature increase of the nanoparticles in the order of 150K. A much higher temperature of the DMAB molecules, around 500K, is regarded as sign of vibrational activation of the molecules by electron injection. The role of the electron injection is corroborated by the observation of an intensity threshold for the photo-driven reaction. On the other hand, a comparison between measurements of the reaction kinetics at different temperatures and different intensities indicate, that an increased reaction rate at higher light intensities could be rooted in a higher temperatures of the particles.

O 8.6 Mon 11:45 H25

Real-space observation of far- and near-field-induced photolysis of molecular oxygen on a Ag(110) surface by visible light — •Chenfang Lin[1] and Takashi Kumagai[1,2] — [1]Department of Physical Chemistry, Fritz-Haber Institute of the Max-Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]JST-PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan

Dissociation of molecular oxygen is an important elementary process in heterogeneous catalysis. Recently, it has been demonstrated that photo-induced dissociation of molecular oxygen can be significantly enhanced using plasmonic Ag nanoparticles and occurs even by visible light via excitation of surface plasmons [1,2]. Here we report the direct observation of oxygen photolysis at low coverages (0.01 monolayer) by far- and near-field excitation in the visible range by using a combination of an STM and a wavelength-tunable laser. It is found that the cross section for the far-field excitation (about 10^{-19} cm^2) can be largely enhanced in a plasmonic STM junction with an Ag or Au tip. We also demonstrate that the wavelength dependence of the oxygen photolysis can be tuned by nanoscale fabrication of an STM tip with focused ion beam milling. Our approach provides a unique opportunity to investigate the optimal nanostructures for plasmonic catalysts.

[1] Phillip Christopher, Hongliang Xin and Suljo Linic, Nature Chemistry 3, 467-472 (2011)
[2] Phillip Christopher, Hongliang Xin, Andiappan Marimuthu and Suljo Linic, Nature Materials 11, 1044-1050 (2012)

O 8.7 Mon 12:00 H25

Colliding Molecules at Selected Impact Parameters — •Kelvin Anggara, Lydie Leung, Matthew Timm, Zhixin Hu, and John Polanyi — Department of Chemistry and Institute of Optical Sciences, University of Toronto, 80 St. George Street, Toronto M5S 3H6, Canada

The dynamics for bimolecular reaction has been elucidated by crossing two molecular beams in the gas-phase under single-collision conditions. The results however have inevitably been averaged over impact parameters - the collision 'miss-distance' - ranging from zero to infinity, obscuring the effect of this important parameter on reaction dynamics. We show that this averaging can be avoided by a aiming a highly-collimated 'projectile' molecule towards a fixed 'target' molecule, with both adsorbed at a surface. Using an electron from the tip of a Scanning Tunnelling Microscope (STM), a single chemisorbed CF_3 on Cu(110) at 4.6 K can be reacted to give a recoiling CF_2 radical that is collimated to a lateral spread of only ±1°. Previous work from this lab has shown that this collimation effect is due to the interaction of the CF_2 with the underlying Cu-row which acts as an atomic guide to give a directed CF_2 'surface-molecular-beam'. Here we have aimed the CF_2 beam at a chemisorbed vinyl ($CHCH_2$) with three impact parameters (-4.0, -0.4, and +3.2 Å), giving insights into the dynamics of carbon chain growth on the metal surface. The scattering experiment presented here has the potential to be aimed at any target that can be detected by STM on a surface, thereby providing a means to explore the dynamics in a wide range of surface reactions.

O 8.8 Mon 12:15 H25

Development of Descriptors for the Prediction of Adsorption Energies on Transition Metal Catalysts and their Alloys — •Martin Deimel, Karsten Reuter, and Mie Andersen — Theoretical Chemistry, Technical University of Munich, Germany

The construction of microkinetic models for catalytic processes requires the knowledge of both adsorption energies of the different species and reaction barriers. In the pursuit of discovering new catalysts with improved activity and selectivity, computational screening renders the explicit calculation from first principles intractable. In order to reduce the computational effort, it is desirable to identify descriptors that allow for a cheap and accurate prediction of these quantities. In the present work we apply the recently developed compressed-sensing method Sure Independence Screening and Sparsifying Operator (SISSO) [1] to identify cheaper and more accurate descriptors for adsorption energies on transition metals (TMs) and their binary alloys [2]. These descriptors are constructed as non-linear functions of properties of the clean catalyst surface (primary features). The different metal atom composition of sites on surface alloys introduces an additional tunable parameter. In combination with distinct site preferences and coordination patterns of different adsorbates, this provides the opportunity to break the interdependence of adsorption energies imposed by scaling relations. Such interdependence is often viewed as one of the major limiting factors for identifying even better catalysts than we know today.

[1] R. Ouyang *et al.*, Phys. Rev. Materials **2**, 083802 (2018)
[2] M. Andersen *et al.*, submitted

Invited Talk O 8.9 Mon 12:30 H25

Deposition and properties of ultrathin films of organic radicals — •Maria Benedetta Casu — Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany

In this work, we demonstrate that it is possible to evaporate and deposit organic radicals onto well-defined surfaces under controlled conditions, without degradation. Using soft X-ray spectroscopies, we investigate thin film processes, surfaces, and interfaces at the nanoscale of organic radicals deposited on metal and metal oxide surfaces. We find that organic radicals are physisorbed and keep their magnetic moment on inert and passivated surfaces, while defective sites such as oxygen vacancies or presence of OH groups lead to chemisorption of the organic radicals on the surface with quenching of their magnetic moment. Our work shows that the use of X-ray based techniques represents a powerful approach to reveal the mechanisms governing complex interfaces, such as radical/metal and radical/metal-oxide where it is important to describe both charge and spin behavior (spinterfaces). A deep understanding of stable radical/inorganic spinterfaces may open the way to use radicals in solid state devices, or as quantum bits with dedicated configurations, as proposed for other molecular quantum bits, and in spin-based electronics.

O 9: Instrumentation Micro-/Nano-Analysis and Lithography/Structuring: Invited Talk Leo Gross (joint session KFM/DS/O)

Time: Monday 15:00–16:30 Location: PHY 5.0.21

Invited Talk O 9.1 Mon 15:00 PHY 5.0.21

On-surface synthesis by atomic manipulation studied with AFM — •Leo Gross — IBM Research - Zurich, Säumerstr. 4, 8003 Rüschlikon, Switzerland

Elusive molecules can be created using atomic manipulation with a combined atomic force/scanning tunneling microscope (AFM/STM). Molecules that are highly reactive and short-lived under ambient conditions can be stabilized at low temperature on inert surfaces. Employing high-resolution AFM with functionalized tips provides insights into the structure, geometry, aromaticity and bond orders of the molecules created and into the reactions performed [1].

We created radicals, diradicals [2], non-Kekulé molecules [3], antiaromatics [4], and polyynes [5] and studied their structural and electronic properties. We recently showed that the reorganization energy of a molecule on an insulator can be determined [6]. In addition, we expanded the toolbox for the synthesis of molecules by atomic manipulation, demonstrating reversible cyclisation reactions [2], skeletal rearrangements [5] and controlled reactions on insulating substrates by electron attachment/detachment [7].

References: [1] L. Gross et al. Angew. Chem Int. Ed 57, 3888 (2018). [2] B. Schuler et al. Nat. Chem. 8, 220 (2016). [3] N. Pavliček et al. Nat. Nano. 12, 308 (2017). [4] Z. Majzik et al. Nat. Commun. 9, 1198 (2018). [5] N. Pavliček et al. Nat. Chem. 10, 853 (2018). [6] S. Fatayer et al. Nat. Nano. 13, 376 (2018). [7] S. Fatayer et al. Phys. Rev. Lett. 121, 226101 (2018).

O 9.2 Mon 15:30 PHY 5.0.21

Additive laser fabrication of silver and silver-composite 3D micro-structures — •Erik H. Waller[1] and Georg von Freymann[1,2] — [1]Physics department and State Research Center OPTIMAS, Technische Universität Kaiserslautern, Kaiserslautern — [2]Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern

We present direct laser writing (DLW) of silver and silver-composite microstructures via photoreduction in liquid resists. Several photoresist compositions are compared based on visual inspection of 2D and 3D test structures complemented by EDS and spectral resonance measurements.

Compared to common approaches for additive manufacturing of 3D metallic structures, e.g., selective laser melting or sintering, DLW is a very precise fabrication technology allowing sub-micrometer feature sizes. However, structures fabricated by DLW are usually made of polymers. Renewed interest in DLW of metallic microstructures has emerged due to their potential, e.g., in plasmonics. The underlying principle of metal DLW is photo-induced reduction of a precursor to neutral metal within the laser focus. The metal particles subsequently agglomerate to form the building block of a structure. Adverse effects are mainly heating of and scattering by the evolving structure as well as low quantum yield and slow speed of the reaction. Thus, we here test different photoresist compositions with respect to the above mentioned criteria and identify key parameters to best control these photoreactions.

O 9.3 Mon 15:50 PHY 5.0.21

Hard X-ray Photoelectron Diffraction in Graphite — •Olena Fedchenko[1], Sergey Chernov[1], Katerina Medjanik[1], Sergey Babenkov[1], Dmitry Vasilyev[1], Aimo Winkelmann[2], Hans-Joachim Elmers[1], and Gerd Schönhense[1] — [1]JGU, Institut für Physik, Mainz — [2]Laser Zentrum, Hannover

A new high-energy momentum microscope (kinetic energies up to >7 keV) allows full-field imaging of the (k_x-k_y) photoelectron distribution with a large field of view (up to 20 $Å^{-1}$ dia.) in momentum space and ToF energy recording. Avoiding symmetry-varying rotation of sample and/or analyser, "full-field k-imaging" provides an ideal means for X-ray photoelectron diffraction (XPD) studies. High-resolution ($< 0.1°$) diffractograms can be recorded within minutes thanks to the high brilliance of beamline P22 at PETRA III [1]. We present an XPD study for electrons from the C 1s core level in graphite in a wide energy range from 2840 to 7283 eV. Fine details in the diffractograms reflect the large number of scatterers (10^5-10^6) due to the large inelastic mean free path. A calculation based on the Bloch wave approach to electron diffraction by lattice planes [2] shows excellent agreement. The short photoelectron wavelength (10% of the interatomic distance) "amplifies" phase differences and turns hard X-ray XPD into a very sensitive structural tool. The results are important for valence band XPD [3].

[1] C. Schlueter et al., Synchr. Radiation News 31, 29 (2018); [2] A. Winkelmann et al., New J. of Phys. 10, 113002 (2008); [3] G. Schönhense et al., arXiv 1806.05871 (2018).

O 9.4 Mon 16:10 PHY 5.0.21

High-Resolution High-Sensitivity Characterization using SIMS based Correlative Microscopy — •Santhana Eswara, Alisa Pshenova, Jean-Nicolas Audinot, and Tom Wirtz — Advanced Instrumentation for Ion Nano-Analytics, MRT, Luxembourg Institute of Science and Technology, L-4422 Belvaux, Luxembourg

Technological materials are being increasingly engineered by optimizing the structure at the nanometer-level and the chemical composition at the dopant-level. Therefore, analytical techniques capable of both high-resolution and high-sensitivity are indispensable. Transmission Electron Microscopy (TEM) offers excellent lateral resolution down to atomic scale, but the analytical techniques typically available in a TEM such as EDX or EELS do not have the sensitivity to analyze trace elements (e.g. dopants). In comparison, Secondary Ion Mass Spectrometry (SIMS) is well-known for high-sensitivity analysis of materials down to the ppm level. However, the lateral resolution of SIMS is fundamentally limited by the ion-solid interaction volume to ˜ 10 nm. Recently we developed SIMS in a Helium Ion Microscope (HIM) and demonstrated a SIMS lateral resolution of ˜ 15 nm[1]. While this is a remarkable breakthrough, it is still 2 to 3 orders-of-magnitude poorer in comparison to high-resolution techniques such as TEM imaging. To overcome this limitation, we developed correlative microscopy methods combining SIMS imaging with high-resolution techniques such as TEM and HIM (SE mode). We will discuss the HIM-SIMS and in-situ TEM-SIMS correlative techniques[2]. [1] D. Dowsett et al, Anal. Chem., 89, 8957-8965, 2017 [2] L. Yedra et al, Sci. Rep. 6, 28705, 2016

O 10: New Methods and Developments II: Scanning Probe, Spectroscopic, and Diffraction Techniques

Time: Monday 15:00–18:00 Location: H3

O 10.1 Mon 15:00 H3

Interaction between a metallic STM tip and a single CO molecule adsorbed on a copper surface — •Norio Okabayashi[1,2], Angelo Peronio[2], Sonia Matencio[2], Ferdinand Huber[2], Thomas Frederiksen[3], Magnus Paulsson[4], and Franz J. Giessibl[2] — [1]Kanazawa University, Kanazawa, Japan — [2]University of Regensburg, Regensburg, Germany — [3]Donostia International Physics Center, San Sebastián, Spain — [4]Linnaeus University, Kalmer, Sweden

In order to investigate the interaction between a CO molecule and the metallic tip of a scanning probe microscope, we have combined inelastic electron tunneling spectroscopy (IETS) and non-contact atomic force microscopy (AFM) with a qPlus sensor. We have found that the higher the tip-molecule interaction, the more the vibrational modes of the molecule are perturbed. These findings have been rationalized by a classical model describing the molecule as a double pendulum, where the presence of the tip weakens the tip-surface chemical bond [1]. However, in our previous research, the lower limit of a tip molecule distance for an IETS measurement was restricted owing to the method to measure a tunneling current with an interaction force. We have improved our method to understand what happens at smaller tip molecule distances, confirming the validity of our previous findings for both the Cu(111) and Cu(110) surfaces. In addition, bistable configurations are observed at very small tip-molecule distances for both surfaces. [1] N. Okabayashi, A. Peronio, M. Paulsson, T. Arai, and F. J. Giessibl, PNAS 115, 4571 (2018).

O 10.2 Mon 15:15 H3

DFT-based forces on a CO tip approaching Fe, Cu, Si adatoms on Cu(111) in an atomic force microscope — •Svitlana Polesya[1], Sergiy Mankovsky[1], Ferdinand Huber[2], Franz Giessibl[2], and Hubert Ebert[1] — [1]Dept. Chemistry, LMU Munich, D-81377 Munich, Germany — [2]Inst. Expt./Appl. Physics, University of Regensburg, 93053 Regensburg, Germany

We present the results of a DFT-based investigation on the forces experienced by a CO tip approaching different types of atoms deposited on Cu(111) surface: Cu, Fe and Si. A similar behaviour has been found for the forces as function of distance of CO molecule from Cu and Fe adatoms: they show two attractive minima with a repulsive 'barrier' in-between. In contrast to this, in case of a Si adatom the force on a CO tip is always repulsive at distances $d \leq 400$ pm from the adatom. These findings are discussed using similar arguments as in the discussion of chemical and physical adsorption on a surface. In particular, attractive forces in the vicinity of Fe and Cu adatoms are explained by the formation of bonding states giving a significant energy gain in these cases, while charge redistribution in the vicinity of Si adatom is responsible for a strong Coulomb repulsion at these distances. Similar arguments are used to explain the variation of the force upon a lateral motion of the tip at constant distance from the surface, that was found in a good agreement with experiment. Based on these results we conclude about the crucial role of the quantum-mechanical contribution to the forces between the Fe and Cu adatoms and a CO tip responsible for experimentally observed AFM image.

O 10.3 Mon 15:30 H3

In-situ characterization of O-terminated copper tips for high-resolution atomic force microscopy — •Alexander Liebig and Franz. J. Giessibl — University of Regensburg, Regensburg, Germany

The use of chemically inert tips allows to directly probe the repulsive interaction regime and thus to obtain high spatial resolution. Gross *et al.* found in 2009 [1] that CO-terminated metal tips enable intramolecular resolution imaging of organic molecules. Later, it was found that terminating the tip apex with noble gas atoms [2] achieves a similar spatial resolution. Recently, Mönig *et al.* [3] proposed to use oxygen-terminated Cu tips that apparently are also quite inert, but are stiffer in lateral directions than CO tips. So far, to verify tip functionalization with oxygen, the STM and AFM contrast of copper oxide domains has been compared to calculated images for different tip models. Here, we apply the COFI method [4] and force spectroscopy to characterize O-terminated Cu tips *in-situ* on a Cu(110) surface. Our approach is an efficient way to experimentally determine both the structural composition as well as the chemical species of the tip apex. Knowledge of these properties is of crucial importance, especially if the tips are used for experiments on other sample systems. The experimental data about the tip structure and composition is expected to improve the precision of theoretical studies about the interaction between tip and sample. [1] L. Gross *et al.*, Science **325**, 1110 (2009). [2] F. Mohn *et al.*, Appl. Phys. Lett. **102**, 073109 (2013). [3] H. Mönig *et al.*, ACS Nano **10**, 1201 (2016). [4] J. Welker *et al.*, Science **336**, 6080 (2012).

O 10.4 Mon 15:45 H3

Atomic-scale inelastic electron tunnelling spectroscopy with superconductive tips — •Angelo Peronio and Franz J. Giessibl — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

Inelastic electron tunnelling spectroscopy with a scanning tunnelling microscope (STM-IETS) enables the measurement of excitations with atomic spatial resolution, such as vibrational and rotational modes of single molecules, and flip of single spins. The intrinsic lineshape of molecular vibrations carries information on the electron-vibration coupling, the hybridization of the molecule with its environment, and the degree of vibrational damping by electron-hole pair excitation. On the other hand, the measured lineshape is usually dominated by extrinsic effects, such as temperature, modulation, and instrumental radiofrequency broadening. The temperature broadening originates form the finite width of the Fermi edge of the electronic density of states of the tip apex. We circumvent the temperature broadening by using the gap of a superconductive STM tip to probe the vibrational modes of carbon monoxide adsorbed on copper, and deconvolving the density of electronic states of the tip from the resulting spectra.

O 10.5 Mon 16:00 H3

Single molecule nanotribology: understanding friction and adhesion at a single molecule level. — •J.G. Vilhena, Remy Pawlak, and Ernst Meyer — Department of Physics, University of Basel

Understanding the motion/dynamics of a single molecule over a surface is a problem of a paramount importance in the design of advanced molecular nanostructures/assemblies capable of meeting specific needs. Nevertheless, to date, understanding the interplay between molecule mechanics, surface displacements and dynamics at a atomic level is a highly challenging task since it requires the knowledge of not only the forces needed to manipulate them but also to relate them with particular molecular/atomic motion. Here we bridge this gap by combining MD simulations, scanning probe microscopy and force spectroscopy to investigate the manipulation of two different molecules (ssDNA and poly-pyrene) over a Au(111) surface in UHV at 5K. Our experiments/simulations revealed a contrasting on-surface dynamics of these molecules. The high ssDNA adhesion to Au(111) enabled us to chart the unexplored nano-Newton tensile force regime which allowed to quantify for the first time the stretching stiffness of a single DNA nucleotide. In the other extreme, the low adhesion and superlubric behavior of the poly-pyrene revealed a surprising complex on-surface dynamics of the molecule. Our simulations/experiments reveal a dynamic balancing between the intra-molecular mechanics and surface comensurability which result in a snake like motion of the molecule over the surface.

O 10.6 Mon 16:15 H3

Sensing in-plane and out-of-plane nanomechanical Surface and Subsurface Properties of Polymers — •Anna Lisa Hawlitschek — TU Darmstadt

Bimodal atomic force microscopy enables the quantitative nanomechanical analysis of heterogeneous polymers. The technique is based on the simultaneous excitation and detection of two different cantilever eigenmodes. Depending on the type of the oscillation modes (flexural or torsional), out-of-plane elastic and dissipative sample properties or the in-plane shear behavior can be analyzed. Here, a trimodal approach was developed where in addition to the first flexural eigenmode, the second flexural eigenmode as well as the first torsional eigenmode were excited. The indentation depth of the tip into the sample surface could be controlled by the first flexural oscillation amplitude used for the topographical feedback. The frequency shifts of the second flexural and the first torsional eigenmode provided measures for the elastic moduli and the shear forces, respectively, using a frequency modulation setup in constant amplitude mode. Thus, dissipative interactions could be derived from the drive amplitudes of the second flexural and the first torsional eigenmodes. It was demonstrated that differences in the elastic behavior in in- and out-of-plane direction can be examined on heterogeneous polymers (elastomeric polypropylene and polystyrene-block-polybutadiene diblock copolymer) using this trimodal approach with high lateral and depth precision.

O 10.7 Mon 16:30 H3

Soft x-ray RIXS-Imaging of thin microstructured VO_2 — •Jan Oliver Schunck[1,2], Florian Döring[3], Benedikt Rösner[3], Jens Buck[1], Sanjoy Mahatha[1], Moritz Hoesch[1], Christian Schüssler-Langeheine[4], Adrian Petraru[5], Hermann Kohlstedt[5], Kai Rossnagel[1,6], Christian David[3], and Martin Beye[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg — [2]Physics Department, Universität Hamburg — [3]Paul Scherrer Institut, Villigen, Switzerland — [4]Helmholtz-Zentrum Berlin — [5]Nanoelektronik, Technische Fakultät, CAU Kiel — [6]Institut für Experimentelle und Angewandte Physik, CAU Kiel

This contribution presents the results of imaging Resonant Inelastic X-ray Scattering (RIXS) measurements performed on vanadium dioxide samples at the soft x-ray synchrotron beamline P04 at PETRA III in Hamburg, where a new experimental setup was employed [1]. Instead of averaging over μm-sized x-ray spot foci on the sample, the incident x-rays were focussed to a vertical line, along which the photon energy varied due to the dispersion of the beamline. Furthermore, an off-axis Fresnel zone plate was employed, dispersing the emitted photon energies in horizontal direction onto a CCD camera while imaging the sample in vertical direction. This enables the in-parallel recording of RIXS maps of emitted intensities depending on incident and emitted photon energies. Additionally, scanning the 1D imaged line focus across the sample in perpendicular direction facilitates the recording of 2D images of electronic properties with a spatial resolution of about 2 μm.

[1] F.Marschall *et al.*, Scientific Reports **7**, *8849* (2017).

O 10.8 Mon 16:45 H3

Using X-Ray Cavities for the Enhancement of RIXS Signal Levels — •Robin Yoël Engel[1], Lars Bocklage[1], Simo Huotari[2], Hasan Yavas[3], Marco Moretti Sala[4], Piter Miedama[1], Gyoergy Vanko[5], Ralf Röhlsberger[1], and Martin Beye[1] — [1]DESY, Hamburg, Germany — [2]Dep. of Phys., University Helsinki, Finland — [3]LCLS, SLAC, Menlo Park, USA — [4]Dep. of Phys., Politecnico di Milano, Italy — [5]Wigner RCP, Budapest, Hungary

While Resonant Inelastic X-ray Scattering (RIXS) is a powerful analytic tool for the analysis of material functionality, achieving adequate signal levels is one of the main challenges for experiments. This difficulty lies in the low probability of the inelastic scattering process (J. Synchrotron Rad. (2018). 25, 580-591) combined with the fact that most spectrometers only cover a small part of the solid angle opposed to the quasi-isotropically emitted fluorescence photons. Here, we show a method to significantly increase signal levels by embedding probe layers, in this case thin iron and iron oxide, into a grown multilayer system, which acts as a resonant cavity at specific incident angles. This brings two advantages: First, the standing waves within the cavity exhibit strongly enhanced electric field amplitudes, thus increasing the total fluorescence yield correspondingly. Further, the cavities resonance condition focuses the fluorescence photons into specific emission angles. This talk presents preliminary results of an experiment performed at the ESRF, demonstrating the expected resonant cavity effects, leading to a five-fold enhancement in signal due to the focusing of fluorescence photons on top of the effect of enhanced excitation.

O 10.9 Mon 17:00 H3

Three-dimensional atomic image reconstruction by means of high kinetic energy electron holography — •Christopher Kohlmann[1,2], Matthias Gianfelice[1], Gert Nolze[3], Lukas Kesper[1,2], Richard Hönig[1,2], and Carsten Westphal[1,2] — [1]Experimental Physics I - TU Dortmund University, Otto-Hahn-Str. 4a, D-44221 Dortmund — [2]DELTA - TU Dortmund University, Maria Goeppert-Mayer-Str. 2, D-44221 Dortmund — [3]BAM, Unter den Eichen 87, D-12205 Berlin

The determination of the atom locations in crystalline structures is of great importance for numerous systems and applications. Without a detailed knowledge of the atomic structure, the creation of synthetic systems with pre-determined properties, or the calculation of electronic properties would not be possible. For structures directly located at the surface, scanning-probe microscopy is an applicable method determining the surface structure.

One way to gain direct information about the three-dimensional structure in the subsurface region is the holographic approach as proposed by D. Gabor in 1948. The small wavelength of the electron wave is perfectly suited for imaging atoms. In the past electron holography was not as successful as imagined.

We present an electron holography method, which is able of three-dimensional atom image reconstruction with chemical sensitivity in the subsurface regime. Furthermore we will present new approaches of data processing for the experimental execution of this method.

O 10.10 Mon 17:15 H3

Total Reflection High-Energy Positron Diffractometer at NEPOMUC — •Matthias Dodenhöft, Artur Elovskii, Sebastian Vohburger, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, 85748 Garching, Germany

Total Reflection High-Energy Positron Diffraction (TRHEPD) has been established as an ideal technique to determine the crystalline structure of topmost and immediate subsurface atomic layers. In contrast to Reflection High-Energy Electron Diffraction (RHEED), TRHEPD features an outstanding surface sensitivity, which stems from the repulsive crystal potential for positrons and the phenomenon of total reflection.

We have developed a new positron diffractometer that is coupled to the high-intensity positron source NEPOMUC (10^9 moderated e^+ per second) at the research reactor FRM II. The setup features UHV down to 10^{-10}mbar, sample temperatures up to 1000°C and a RHEED system for complementary measurements. The positron beam is accelerated and focused by an electrostatic lens system. We simulated the particle trajectories to optimize the beam properties in order to obtain a parallel, slightly converging beam with a small diameter of around 1mm. First experimental results are expected in spring 2019.

The project has been supported by the BMBF (funding number 05K16WO7).

O 10.11 Mon 17:30 H3

Graphene-Enhanced Raman Spectroscopy of CoOEP molecules — •Simon Rauls, Stephan Sleziona, Tobias Foller, Leonhard Christen, Phillip Ernst und Marika Schleberger — Universität Duisburg-Essen, AG Schleberger, Germany

Graphene-enhanced Raman spectroscopy (GERS) has been shown to be a powerful tool for ultra-sensitive detection of adsorbed molecules [1]. As a possible mechanism charge transfer is often suggested, which depends on the Fermi-level of the graphene, the HOMO-LUMO levels of the molecules and the excitation laser energy [2, 3]. Therefore, a combination of changing the fermi level in a graphene-based field effect device (GFET) and the excitation laser energy is tempting. To exploit this approach several methods have to be combined: (i) preparation of the GFET by photolithography, (ii) controlled deposition of molecules and characterization by measuring the interplay of the transport characteristics and Raman spectra of (iii) the pristine device and (iv) after deposition of molecules. We will present first results from evaporated Cobalt Octaethylporphyrin (CoOEP). This system allows to investigate if the magnetic properties of the molecule may be manipulated with the help of the GFET through Coulomb or quantum mechanical coupling [4].

[1] X. Ling et al., Small, 6 (2010), pp. 2020*2025
[2] E.B. Barros et al., Phys. Rev. B, 90 (2014), 035443
[3] Q. Hao et al., Appl. Phys. Lett., 102 (2013), 011102
[4] C. Crevetti et al., Nat. Mater., 15 (2016), pp. 164*168

O 10.12 Mon 17:45 H3

Probing atomic site-specific electronic and catalytic properties of bimetallic surfaces by tip-enhanced Raman spectroscopy — •Jinhui Zhong[1,2], Hai-Sheng Su[1], Xi Jin[1], Xia-Guang Zhang[1], De-Yin Wu[1], and Bin Ren[1] — [1]State Key Laboratory of Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen 361005, China — [2]Institute of Physics, Carl von Ossietzky University Oldenburg, 26129 Oldenburg, Germany

Revealing site-specific electronic and catalytic properties of catalysts is highly desirable for an atomic and molecular level understanding of heterogeneous catalysis. We demonstrated the use of tip-enhanced Raman spectroscopy (TERS) to chemically and spatially resolve site-specific electronic and catalytic properties of bimetallic catalyst surfaces [1,2]. We first investigated an atomically well-defined Pd(submonolayer)/Au(111) bimetallic model catalyst surface using phenyl isocyanide as a probe molecule. We obtained local nanospectroscopy at a spatial resolution of 3 nm in real space, which revealed a weakened NC bond and enhanced reactivity of phenyl isocyanide adsorbed at the Pd step edge compared with that at the Pd terrace site. We further studied a sub-10 nm sized Pt nanoisland deposited on Au(111) surface. Site-specific properties of Au terrace, Pt terrace, step edge, corner and kink sites with varying coordination numbers on the Pt nanoisland/Au(111) bimetallic surface were observed. Our results pushes important steps towards the (in-situ) probing and understanding of local structure correlated catalytic activity and selectivity of real catalysts at truly atomic and molecular level.

O 11: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge II (joint session O/TT/DS/CPP)

Time: Monday 15:00–17:30 Location: H9

O 11.1 Mon 15:00 H9

Influence of structural deformations on the applicability of the Tamm-Dancoff approximation for organic molecules — •Tobias Lettmann and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

When calculating excited state properties of electronic systems within the many-body perturbation theory (MBPT), the Bethe-Salpeter equation (BSE) needs to be solved. This is often done within the Tamm-Dancoff approximation (TDA), neglecting the coupling of resonant and anti-resonant excitations.

It is generally accepted that the TDA is justified for large, extended systems e.g. bulk crystals. However it has been shown that the TDA may no longer hold for small organic molecules [1]. In this talk we discuss the applicability of the TDA for molecules of different sizes and show the transition between the two regimes. We then discuss how the applicability is influenced by deformations of the molecules, in particular by the related conjugation length of the π-system.

[1] B. Baumeier et al., J. Chem. Theory Comput. **8**, 997 (2012)

O 11.2 Mon 15:15 H9

Momentum-Resolved Electron Energy-Loss Spectroscopy in Oxides from Many-Body Perturbation Theory — •Christian Vorwerk[1,2], Caterina Cocchi[1,2], and Claudia Draxl[1,2] — [1]Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]European Theoretical Spectroscopy Facility

Electron energy-loss spectroscopy (EELS) is a powerful tool to investigate the local electronic and structural properties of crystalline materials. The accurate determination of these spectra from first principles requires a reliable description of the electron-hole interaction, screened by the surrounding many-electron system. We perform *ab initio* many-body perturbation theory calculations of EELS through the solution of the Bethe-Salpeter equation (BSE), including the screened non-local interaction between electron and hole. Employing an implementation in the all-electron full-potential package `exciting`, we show results for a wide range of energy loss, from the optical to the hard x-ray region. We study EELS at finite momentum loss $\mathbf{q}$, from small $\mathbf{q}$ close to the dipole limit to large $\mathbf{q}$ well beyond the first Brillouin zone. This momentum resolution of EELS reveals dipole-forbidden excitations that are invisible in absorption spectroscopy. Our calculations also yield insight into the excitonic dispersion, *i.e.* the excitonic bandstructure. We discuss the effects of momentum loss in the EELS spectra of oxide materials, including CaO, CeO_2, and the wide-gap transparent oxide Ga_2O_3, considering both the optical and x-ray energy-loss range.

O 11.3 Mon 15:30 H9

Electron-magnon scattering in elementary ferromagnets from first principles: implementation and results — •Christoph Friedrich, Mathias C.T.D. Müller, and Stefan Blügel — Peter Grünberg Institut and Institute of Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Propagating electrons and holes can scatter with spin fluctuations and form quasiparticles as a result or more complex many-body states. To calculate this effect, a **k**-dependent self-energy describing the scattering of electrons and magnons is constructed from the solution of a Bethe-Salpeter equation for the T matrix. Partial self-consistency is achieved by the alignment of the chemical potentials. We discuss details of the implementation and illustrative results. The renormalized electronic band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy, which are strongest in Fe. The renormalization gives rise to a band anomaly at large binding energies in iron, which results from a coupling of the quasihole with Stoner excitations.

O 11.4 Mon 15:45 H9

Dielectric function of homogeneous electron gas from Bethe-Salpeter equation — •Jaakko Koskelo[1,2], Martin Panholzer[2,3], Lucia Reining[1,2], and Matteo Gatti[1,2,4] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, F-91128 Palaiseau, France — [2]ETSF — [3]Institute for Theoretical Physics, Johannes Kepler University, Linz, Austria — [4]Synchrotron SOLEIL, France

The homogeneous electron gas (HEG) is one of the most important model systems in condensed matter physics, and it has been subject of a great number of studies. Some properties of HEG such as total energy and static correlation functions can be obtained from quantum Monte Carlo simulations with great accuracy, but for dynamical correlation functions only very few results are available.

Methods based on the Bethe-Salpeter equation (BSE) have been very succesful in semiconductors and insulators, but metals have been less studied. In this contribution, we use the BSE in its standard approximations, including a statically screened electron-hole interaction, to study the dielectric function of HEG. We find significant differences in static screening and spectra compared to other approaches. In particular, the BSE in its current approximations fails to reproduce the negative static screening in the low-density HEG, which is related to a so-called ghost exciton. We also use the time-dependent mean-density approximation [1] in order to compare our results to experimental loss spectra of sodium.

[1] M. Panholzer et al, Phys. Rev. Lett. **120**, 166402 (2018).

O 11.5 Mon 16:00 H9

DFT study of electronic and optical properties of SrTiO$_{3-\delta}$ including many-body effects — •Vijaya Begum, Markus E Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg.

The electronic and optical properties of SrTiO$_3$ (STO), a perovskite material of key importance in the field of oxide electronics, are explored in the framework of density functional theory including many-body effects within the GW approximation and excitonic corrections by solving the Bethe-Salpeter equation (BSE). We further analyse the origin of the strong excitonic effects, in particular a peak at ≈6.5 eV, by decomposing the BSE eigenvectors obtained from GW+BSE to extract the leading electron-hole pair contribution for the particular BSE eigenstate following the approach of Bokdam *et al.* [Scientific Reports 6, 28618 (2016)]. Alternatively, we use the model-BSE (mBSE) which utilises a parametrised analytical model for the static screening. For STO, the mBSE spectrum closely reproduces the one from GW+BSE, which allows to reduce the computational effort by circumventing the intermediate time-consuming GW step. We further proceed to describe the effect of oxygen defects on the electronic and optical properties in STO.

Funding by DFG- SFB1242, project C02 is gratefully acknowledged.

O 11.6 Mon 16:15 H9

Second-order Møller-Plesset perturbation theory and beyond for the band gap and single-particle excitations of solids — •Maria Dragoumi[1], Sergey V. Levchenko[2,1,3], Igor Ying Zhang[4,1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE — [2]Skolkovo Innovation Center, Moscow, RU — [3]NUST MISIS, Moscow, RU — [4]Fudan University, Shanghai, CN

Calculations of the fundamental band-gap and the low-energy excitations of solids are still a challenge for electronic-structure theory. The computationally efficient Kohn-Sham (KS) density functional theory (DFT) with the widely used local or semi-local approximations provides a KS band gap which is much smaller than the fundamental gap. Many-body perturbation theory, on the other hand, addresses the fundamental gap directly. We present here an efficient scalable implementation of Møller-Plesset second order perturbation theory (MP2) for quasi-particle energies [1,2]. By solving the Dyson equation of the single-particle Green's function, considering self-energy up to second order, we go beyond MP2. The new approach shows a competitive or even superior performance in comparison to the current state-of-the-art methods such as hybrid functionals and GW approximation, where second order exchange is missing. We present numerical results for the band-gap of a wide range of semiconductors and insulators.

[1] J. Sun and R. J. Bartlett, J. Chem. Phys. 104, 8553 (1996).

[2] A. Grüneis, et.al, J. Chem. Phys. 133, 074107 (2010).

O 11.7 Mon 16:30 H9

Accelerating *GW* Calculations within the LAPW Framework — •Sven Lubeck, Andris Gulans, and Claudia Draxl — Humboldt-Universität zu Berlin, Germany

The GW approach of many-body perturbation theory is an indispensable method for calculating the electronic band structure of solids. Its implementation in computer programs using the linearized augmented plane-wave + local orbital (LAPW+LO) method allows for obtaining numerically precise results. Unfortunately, high precision comes at the price of a large number of LAPWs and LOs. In this work, we accelerate GW calculations by optimizing the use of LAPWs and LOs in the computer package `exciting` [1]. On the one hand, we introduce a systematic way of obtaining a minimal set of LOs. On the other hand, we perform a basis transformation from the plane-wave part of the LAPWs to different types of basis functions, exploring the efficiency of numeric atom-centered orbitals, Gaussian type orbitals, and Kohn-Sham orbitals. Presenting band gaps of two exemplary materials, zincblende ZnO and hexagonal monolayer BN, we illustrate that our optimization schemes reduce the computational cost down to values as low as 15% without compromising the precision.

[1] 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).

O 11.8 Mon 16:45 H9

Ab-initio description of transient ion formation of NO on Au(111) — Daniel Corken, Nicholas D. M. Hine, and •Reinhard J. Maurer — Departments of Physics and Chemistry, University of Warwick, United Kingdom

Gaining a fundamental understanding of the interactions of molecules on metal surfaces is essential for the development of novel heterogeneous catalysts. An interesting feature of gas-surface reactions at metal surfaces is that the Born-Oppenheimer approximation breaks down. Vibrationally excited and translationally hot molecules can transfer energy to the electrons of a metal via excitation of electron-hole pairs (EHP). In case of NO on Au(111), [1] this nonadiabatic energy loss is believed to stem from the transient generation of charged ion species at the surface. A computationally feasible and accurate description of such a molecule-metal charge-transfer state represents a challenge and several methods have been proposed. Upon a review of existing experimental evidence, we will present our approach to this problem. We use linear expansion-Delta-Self-Consistent-Field Density Functional Theory (leΔSCF-DFT) [2] to model the anionic resonance of NO on Au(111). The leΔSCF-DFT method enforces the electronic configuration of reference molecular states while solving the Kohn-Sham equations self-consistently. By comparison to experiment and other models, we asses the methods' ability to describe the ground- and excited-states during molecular scattering. We further explore avenues to extract nonadiabatic couplings and to construct model Hamiltonians based on this method. [1] JCP 130, 174716, [2] JCP 139, 014708;

O 11.9 Mon 17:00 H9

Luminescence of β-SiAlON:Eu^{2+} phosphors: DFT study — •Saleem Ayaz Khan[1], Ondrej Sipr[1], Robin Niklaus[2], Wolfgang Schnick[2], and Jan Minar[1] — [1]University of West Bohemia, Pilsen, Czech Republic — [2]LMU Munich, Germany

Highly efficient phosphor-converted light-emitting diodes (pc-LEDs)are popular in lighting and high-tech electronics applications[1]. Among them β-SiAlON:Eu^{2+} stands out as a promising narrow-band green phosphor for white-LEDs applications exhibiting good thermal and chemical stabilities. Photoluminescent properties of this material can be tuned by introducing the disorder at various sublattices. To understand the mechanism behind this effect, we performed a systematic study of electronic structure and photoluminescence properties of β-SiAlON:Eu^{2+}. The calculations were done within the *ab-initio* fully relativistic full-potential framework. The disorder was treated by employing both the supercell approach and the coherent potential approximation (CPA). The Stokes shifts were calculated from differences of total energies of the ground and excited states of β-SiAlON:Eu^{2+}. The main focus is on monitoring how the Al and O content and Eu^{2+} activator concentrations influence the local β-Si3N4 electronic structure and how this may be used to tune photoluminescence properties.

[1] Z. Wang, W. Ye, Iek-H. Chu, and S. P. Ong, Chem. Mater., **28**, 8622 (2016).

O 11.10 Mon 17:15 H9

Spin fluctuations in itinerant ferromagnets: Computing the dynamic transverse spin susceptibility with TDDFT and PAW — •Thorbjørn Skovhus and Thomas Olsen — Technical University of Denmark

We present a numerical scheme for computing the dynamic transverse spin susceptibility using time-dependent density functional theory which allows us to study magnons in itinerant ferromagnets. The scheme is based on a real-space grid implementation of the projected augmented wave method and use a simple plane wave representation of the response function. Employing the adiabatic local density approximation for the exchange-correlation kernel, calculations of the magnon spectra in bulk transition metals iron and nickel are presented. In the context of the present implementation, the influence from the choice of numerical scheme on the violation of the Goldstone theorem is investigated.

O 12: Nanostructures at Surfaces II: Designer Structures and Surfaces

Time: Monday 15:00–17:45 Location: H15

Invited Talk O 12.1 Mon 15:00 H15

Nanoscale engineering at surfaces — •F Stefan Tautz — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — Jülich Aachen Research Alliance (JARA), Fundamental of Future Information Technology, 52425 Jülich, Germany — Experimental Physics IV A, RWTH Aachen University, 52074 Aachen, Germany

The increasing interest in quantum technologies puts tailor-made materials into the focus. In this context the term material is more and more understood in a wider sense to also include designer structures beyond a single crystalline phase. For example, such designer structures can be customized stacks of 2D materials as well as surface-supported nanostructures made by assembling individual atoms or molecules. A further challenge, apart from crafting the structures, is studying their properties. Often, this requires the refinement of existing experimental methodologies. In my talk, I will report on our recent work regarding tailor-made materials based on graphene and designer structures based on individual atoms and molecules. With increasing complexity, new properties and phenomena emerge, and the design of functional (quantum) devices becomes possible. As it turns out, even relatively simple designer structures show intriguing functionalities, including quantum dot behaviour, electrostatic potential sensing, and coherent single-electron field emission. On the analytic side, I will illustrate the power of several advanced experimental methodologies.

O 12.2 Mon 15:30 H15

The electrostatic potential of atomic chains and clusters imaged quantitatively with scanning quantum dot microscopy — Philipp Leinen[1,2], •Rustem Bolat[1,2], Ruslan Temirov[1,2], F. Stefan Tautz[1,2], and Christian Wagner[1,2] — [1]Peter Grünberg Institut (PGI-3), Jülich, Germany. — [2]JARA-Fundamentals of Future Information Technology

Fabrication of artificial atomic clusters and chains facilitates the observation and investigation of various quantum effects. The size and geometry of such assemblies influence electrostatic potentials, catalytic efficiency as well as a magnetic response. Here, we investigate the electrostatic properties of differently sized and shaped Ag clusters which have been created on a Ag(111) substrate by atomic manipulation with a scanning probe microscope (SPM). We use scanning quantum dot microscopy (SQDM) [1,2] with a single molecule quantum dot attached to the SPM tip [3] to image the surface potential over atomic chains and compact clusters. These potentials originate from the Smoluchowski effect and influence, e.g., the local reactivity. We find that the surface dipole moment per adatom drops rapidly for compact assemblies while it converges to a value of about 0.26 Debye for atoms in a chain.

[1] C. Wagner, et al. Phys. Rev. Lett. 115, 026101 (2015)
[2] M. Green, et al. Japan. J. Appl. Phys. 55, 08NA04-7 (2016)
[3] R. Temirov, et al. Phys. Rev. Lett. 120, 206801 (2018)

O 12.3 Mon 15:45 H15

Low temperature chemical vapor deposition of ZnO nanowire arrays for field emission applications — •Carina Hedrich, Stefanie Haugg, Robert H. Blick, and Robert Zierold — Center for Hybrid Nanostructures (CHyN), Universität Hamburg, Luruper Chaussee 149, 22607 Hamburg, Germany

In the last years, ZnO nanostructures of many different morphologies have been fabricated by various physical and chemical methods and several applications have been realized. Arrays of one-dimensional ZnO nanostructures are promising candidates for electron field emission devices due to their high aspect ratio and low work function of the material. To tailor the synthesis of ZnO nanowires, the influence of the growth parameters on the properties of the nanostructures have to be known. Here, we report about a comprehensive morphology study of ZnO nanowire arrays grown by low temperature (500 -650 °C) chemical vapor deposition as a function of the process parameters. The vapor transport growth was conducted by utilizing zinc acetylacetonate hydrate and oxygen as precursors. The electron field emission characteristics of optimized ZnO nanowire array devices are investigated, by measuring the electron tunnel current as a function of the applied voltage, using a home-made electron field emission setup. Analysis of the field emission data reveal the potential of our nanostructures for tailor-made electron field emission devices. In the future, such ZnO nanowire arrays on silicon nitride membranes might pave the way for advanced detector technologies used in time-of-flight mass spectrometry of proteins with much higher mass resolution than nowadays accessible.

O 12.4 Mon 16:00 H15

X-ray Photoelectron Diffraction and Spectroscopic Investigation of Near-Surface Alloying of Cu/Au(111) — •David Batchelor[1], Federico Grillo[2], Rory Megginson[2], Matthias Muntwiler[3], and Christopher J. Baddeley[2] — [1]KIT, Karlsruhe, Germany — [2]University of St Andrews, St. Andrews, United Kingdom — [3]PSI, Villigen, Switzerland

Binary metal alloys have been, and are, the subject of much investigation. The Copper/Gold System is one such well studied bulk system. The solid alloy is completely miscible over the whole concentration range and a large temperature region, only becoming ordered at low temperature (≈650K). In comparison there are relatively few Surface studies. Recently, it has been demonstrated using STM [1,2] that ordered Surface structures can be grown for this system. To investigate the structures further a Synchrotron Radiation and STM study on the PEARL beamline [3] at the SLS was undertaken. X-ray Photoelectron diffraction was chosen as method as it is not only sensitive to the Surface but also buried layers. In addition to the geometric structure data electronic state information from both valence and core levels was obtained. The data will be discussed together with the results of calculations and modelling.

[1] F. Grillo et al., New J. Phys., 13, 013044 (2011)
[2] F. Grillo et al., e-JSSNT, 16, 163 (2018)
[3] M. Muntwiler et al. J. Synchrotron Rad. 24, 354 (2017)

O 12.5 Mon 16:15 H15

Femtosecond laser generation of microbumps and nanojets on single and bilayer Cu/Ag thin films — •Aida Naghiou[1], Miao He[2], Jasmin S. Schubert[1], Leonid V. Zhigilei[1,2], and Wolfgang Kautek[1] — [1]University of Vienna, Department of Physical Chemistry, Vienna, Austria — [2]University of Virginia, Department of Materials Science and Engineering, Charlottesville, Virginia, USA

Femtosecond laser ablation of metal thin films has been of vivid interest since decades. The generation of microbumps and nanojets have been observed in many studies. It is generally accepted that frozen nanojets are produced through rapid melting. However, the mechanism for the formation of microbumps, is still under discussion. Subsurface boiling and pressure of the vapor released at the substrate-film interface, melting and redistribution of molten material, and plastic deformation of the irradiated film have been suggested as the processes responsible for the generation of the microbumps. In this study, the mechanisms of the formation of microbumps and nanojets on Ag/Cu thin films and double layers irradiated by a single 60 fs laser pulse are investigated experimentally and with atomistic simulations. The composition of the laser-modified bilayers is probed with the energy dispersive X-ray spectroscopy. The simulations reveal the important role of the difference in the electron-phonon coupling factor of the two metals in the mechanism of bump formation and breaching. The computational predictions of the threshold fluences for the formation of microbumps exposing different component of the bilayer targets, and the conditions for the bump breaching, agree well with experimental observations.

O 12.6 Mon 16:30 H15

Structural and electronic characterization of Eu-doped Bi_2Te_3 epitaxial films — •Celso I. Fornari[1], Hendrik Bentmann[1], Thiago R. F. Peixoto[1], Paulo Rappl[2], Eduardo Abramof[2], Sérgio Morelhão[3], Martin Kamp[4], and Celso Fornari[1] — [1]Experimentelle Physik VII, Würzburg — [2]Instituto Nacional de Pesquisas Espaciais, Brazil — [3]Universidade de São Paulo, Brazil — [4]Physikalisches Institut, Würzburg

Bismuth telluride is a simple model for three-dimensional topological insulators (TIs) with a single Dirac cone at the surface. The topological surface states are protected against backscattering due to small imperfections in the lattice or from scattering due to non-magnetic impurities by time reversal symmetry (TRS). However, to unlock novel physical phenomena, it is a prerequisite to break TRS. In this sense, TIs have been investigated by doping with transition metals or rare earth elements and by proximity effect to magnetic layers or substrates.

In this work, we report on a systematic study of the MBE growth of europium doped bismuth telluride films on (111) BaF_2. The small lattice mismatch (0.04 %) to bismuth telluride makes this material a suitable substrate to grow high-quality thin films. Films with nominal Eu concentration ranging from 0 (reference) up to 9 % were produced. Using high-resolution X-ray diffraction (HR-XRD), transmission electron microscopy (TEM) and angle-resolved photoemission spectroscopy (ARPES), evidences of Eu entering Bi sites up to concentrations around 4 % were obtained with a preserved Dirac cone at the surface.

O 12.7 Mon 16:45 H15

Characterization of the optical Kerr-Effect in $CsPbBr_3$-perovskite films — •Daniel Frese[1], Linghai Meng[2], Haizheng Zhong[2], and Thomas Zentgraf[1] — [1]Universität Paderborn, Warburger Str. 100, 33098 Paderborn — [2]Beijing Institute of Technology, Beijing, China

Halide perovskites, like $CsPbBr_3$, have received a lot of attention lately, because of their optical and electronic properties. For example, perovskites have a tunable bandgap and excitons can exist at room temperature, which makes them promising candidates for applications in photovoltaic and electro optical devices. Here, we investigate the optical Kerr-Effect by studying the nonlinear refractive index and nonlinear absorption of $CsPbBr_3$, using the z-scan technique with femtosecond pulsed excitation. The high third-order nonlinearity of thin film perovskites opens up new possibilities in nonlinear optical applications, like nanoscale frequency conversion, wave-mixing, nonlinear holography, and all-optical switching.

O 12.8 Mon 17:00 H15

Revealing the influence of structural disorder in plasmonic systems — •Ediz Herkert, Florian Sterl, Steffen Both, Thomas Weiss, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569, Stuttgart, Germany

In the vast majority of studies, ensembles of plasmonic nanostructures are modeled as identical particles arranged in a perfectly periodic fashion. Several algorithms can efficiently calculate the optical response of these ideal systems. However, in all experiments structural disorder is present due to imperfections in the manufacturing process. This disorder is in fact expected to influence the optical properties. We investigate how disorder affects the optical response and how by the same token disorder can be utilized to tune the optical properties of the plasmonic ensemble. To this end, we define parameters that allow us to control the correlation and randomness of the structures and implement a coupled dipole model to compute the far-field response of any configuration of nanostructures. We validate these simulations with a microscopy setup that provides spectrally resolved real- and Fourier-space images of the plasmonic systems. Based on this data we explore the correlations between the disorder parameters and the optical spectra as well as the optical color appearance. Eventually, we aim to deduce the microscopic structural disorder solely from the measured far-field optical response of the plasmonic structures and tailor ab initio the bidirectional reflection distribution function.

O 12.9 Mon 17:15 H15

Nanostructuring new optical materials using BCML and RIE methods — •Louise Kaeswurm, Zhaolu Diao, Klaus Weishaupt, and Joachim Spatz — Max-Planck-Institute for Medical Research, Department of Cellular Biophysics, Jahnstr. 29, 69120 Heidelberg

To improve the optical properties of silica glass, moth-eye inspired nanostructures etched into the surface of silica glass have shown promising results in reducing the reflectance and increasing the transmittance over 99.5 %. To create these moth-eye structures, an etching mask is applied to the sample via micellar block copolymer lithography (BCML) and pillars are etched into the substrate in a reactive ion etching process.

With this method the performance for a rather large spectral range is increased and the effect is not restricted to a small angular range. Since many other glasses and materials would also profit from such a treatment, current research is focused on the transfer of these techniques to other materials, for example, etching these nanostructures into sapphire, diamond or borosilicate glass. One challenge of these new materials is finding a way to etch very hard or chemically inert structures or irregular structures such as found in borosilicate glass. For this, new etching procedures had to be developed. Another challenge is the cleaning of the substrates without destroying the fragile nanostructure. Here, common ultrasonic cleaning methods did not give convenient results and therefore, megasonic cleaning was tested and optimized.

O 12.10 Mon 17:30 H15

Development of Nanoporous & Mesoporous materials for Environmental Applications — •Chamila Gunathilake — Department of Chemical & Process Engineering, University of Peradeniya, Sri Lanka

Mesoporous silica & carbon materials with various organic pendant groups were developed for interesting applications including high temperature carbon dioxide (CO2) sequestration from power plant, treatment of wastewater streams, uranium extraction from seawater. Research is mainly focused on the incorporation of metal (aluminum, zirconium, calcium, and magnesium) species into mesoporous silica materials with organic pendant (amidoxime) and bridging groups (isocyanurate, benzene) for CO2 capture at elevated temperatures (60, 120 oC). All these hybrid materials synthesized by co-condensation followed by EISA showed high CO2 uptake at elevated temperature (60, 120 oC) reaching the CO2 sorption capacities in the range of 2.15-4.71 mmol/g. Mesoporous silica materials with diethylphosphatoethyl groups (DP-MS) and hydroxyphosphatoethyl pendant groups (POH-MS) were prepared for lead ions adsorption. High affinity of hydroxyphosphatoethyl groups toward lead ions (Pb2+) makes the POH-MS materials attractive sorbents for lead ions, which is reflected by high lead uptake reaching 272 mg of Pb2+ per gram of POH-MS. Amidoxime-modified ordered mesoporous silica (AO-OMS) materials are also attractive sorbents for uranium recovery as evidenced by very high uranium uptake reaching 57 mg of uranium per gram of AO-OMS under seawater conditions.

O 13: Solid-Liquid Interfaces I: Electrocatalysis and Photoelectrochemistry

Time: Monday 15:00–17:30 Location: H16

O 13.1 Mon 15:00 H16

Operando studies of well-defined Co oxide films for OER catalysis with surface X-ray diffraction — •Tim Wiegmann[1,2], Finn Reikowski[1], Firas Faisal[4], Manon Bertram[4], Jakub Drnec[2], Fouad Maroun[3], Jörg Libuda[4], and Olaf Magnussen[1] — [1]Christian-Albrechts-Universität, 24118 Kiel, Germany — [2]European Synchrotron Radiation Facility, 38000 Grenoble, France — [3]Ecole Polytechnique, 91128 Palaiseau, France — [4]Friedrich-Alexander-Universität, 91054 Erlangen, Germany

Transition metal oxides have recently received great attention as highly active, noble-metal-free catalysts for the oxygen evolution reaction (OER), which is a key reaction in electrochemical water splitting. To establish the relationship between their structure and catalytic activity, we conducted operando surface X-ray diffraction (XRD) studies on epitaxial Co_3O_4(111) thin films prepared by different methods. In addition to grazing incidence XRD, transmission surface XRD, a novel technique for fast capture of in-plane surface structure, was employed. For Co_3O_4 films electrodeposited as 3D islands on Au(111) and Au(100), a potential-dependent, reversible change of bulk lattice constant as well as the formation of a nm-thin skin layer can be observed over a wide potential range before the onset of OER. In comparison, smooth films grown in UHV on Ir(100) are structurally stable while exhibiting a much lower catalytic performance. The influence of the films' granular morphology on their behaviour in the pseudo-capacitive regime and catalytic activity will be discussed.

O 13.2 Mon 15:15 H16

In operando surface X-ray diffraction studies of Co oxide catalysts films for electrochemical water splitting — •canrong qiu, finn reikowski, olaf magnussen, and jochim stettner — Christian-Albrechts-Universität zu Kiel, Institut für Experimentelle und Angewandte Physik, Leibnizstraße 19, 24118 Kiel

Transition metal oxide have been receiving much recent interest as active and stable electrocatalysts for the anodic oxygen evolution reaction (OER). We present operando surface X-ray diffraction studies of two structurally well-defined epitaxial Co3O4(111) and CoOOH(001) films electrodeposited on Au(111). The potential-dependent structural changes were monitored with high time resolution up to OER current densities as high as 150 mA cm 2. The CoOOH(001) film is found to be smooth and perfectly stable over a wide potential range. In the case of Co3O4(111), fast and fully reversible structural changes are observed. The surface region of Co3O4(111) starts restructuring at potentials 300 mV negative of the onset of the OER, indicating that the process is related to the thermodynamically predicted Co3O4 /CoOOH(001) transition. The formed skin layer changes linearly with applied potential. The results are at variance with previous suggestions that di-*-oxo bridged Co cations are exclusively responsible for the OER activity of Co oxides.

O 13.3 Mon 15:30 H16

Overpotentials of the Oxygen Evolution Reaction on Rutile TiO_2: Effect of the Solvent — •Patrick Gono, Francesco Ambrosio, and Alfredo Pasquarello — *Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

We investigate the solvation effect of water on the overpotentials of the oxygen evolution reaction on rutile TiO_2 through first-principles density functional theory calculations. Applying the thermodynamic integration method on an atomistic semiconductor-water interface, we calculate the free energy steps corresponding to the oxygen evolution reaction treating the solvent explicitly. These results are compared with those achieved by employing a computational method in which solvent effects are neglected. The modifications in the free energy steps are analysed in terms of hydrogen bonds between adsorbates and the water molecules of the solvent, as well as the electronic structure of the reaction intermediates.

O 13.4 Mon 15:45 H16

Modelling cost-effective RuO_2 catalysts for the electrochemical oxygen evolution reaction via a core-shell approach — •Yonghyuk Lee, Daniel Opalka, Christoph Scheurer, and Karsten Reuter — Technische Universität München

Rutile-type transition metal oxides such as RuO_2 and IrO_2 currently receive great attention due to their high catalytic activity for the oxygen evolution reaction (OER) in acidic electrolytes. While most OER catalysts in proton exchange membrane electrolyzers rely currently on expensive IrO_2 catalysts due to their favorable stability, RuO_2 shows even higher activity at substantially reduced costs. In the present work, we explore a core-shell approach coating RuO_2 on lattice-matched rutile oxides to potentially yield highly active, relatively inexpensive and chemically stable catalyst materials for water electrolysis. For a first characterization of RuO_2 surfaces, we employed *ab initio* thermodynamics and the computational hydrogen electrode model to determine relative stabilities of pristine and hydrated surfaces as a function of applied potential. Relevant RuO_2 structures at OER operating conditions are compared to core-shell designs, and key factors which further stabilize the system are discussed. Finally, we present thermodynamic reaction barriers for anodic water oxidation and illustrate potential OER pathways that demonstrate enhanced OER activity at surfaces of core-shell materials.

O 13.5 Mon 16:00 H16

A Kinetics-Based Computational Catalyst Design Strategy for the Oxygen Evolution Reaction on Transition Metal Oxide Surfaces — •Simeon D. Beinlich[1], Craig P. Plaisance[2], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Louisiana State University, USA

Aiming to extend over prevalent thermodynamical models, we present a catalyst design strategy for the oxygen evolution reaction (OER) at transition metal oxide (TMO) surfaces that explicitly considers aspects of the reaction kinetics. This strategy is based on extensive DFT+U calculations for a large number of doped active sites on three different surface terminations of cobalt(II,II) oxide.

On this basis, we adapt existing Brønstead-Evans-Polanyi relationships to achieve an accurate description of the two-step nature of the rate-limiting water addition step in the OER. This reveals that the electrochemical and nonelectrochemical pathways of water addition are kinetically equivalent under certain conditions. It also yields a simplified kinetic model to derive a generalized expression for the catalytic activity. We use this model to formulate design criteria for optimal catalytic performance, which pose structure-sensitive and electrode-potential-dependent restrictions for the oxidation potentials of the metal centers involved in the reaction.

The kinetics-based design strategy as well as these design criteria are expected to be transferable to other TMOs and similar electrocatalytic systems dominated by kinetic barriers.

O 13.6 Mon 16:15 H16

Kinetic and transport effects in the ORR on Pt/Ru(0001) model catalysts — •Albert K. Engstfeld, Klein Jens, Fuchs Stefan, Jusys Zenonas, and R.Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The efficiency of a fuel cell (fueled with, e.g., H2, MeOH) could be enhanced by decreasing the overpotential for the oxygen reduction reaction (ORR) at the cathode at low current densities (kinetic limitations). At high overpotentials (high current densities), the reaction is mass transport limited and thus only depends on the geometric arrangement as well as the loading of the active catalyst material. In this work, we report on the ORR on monolayer high Pt island modified Ru(0001) model electrodes. The surfaces are prepared and characterized by STM under UHV conditions, while the electrocatalytic investigation is performed in an electrochemical flow cell system attached to the main UHV system.[1] We will first discuss the influence of the Pt coverage on the kinetic currents and show that electrodes with high Pt coverages are more active than bare Pt(111). Second, we demonstrate that at high overpotentials electrodes with low Pt coverages show a much larger turn-over frequency per Pt atom compared to high Pt coverages. Finally, we observed that our model catalyst also forms significant amounts of H2O2. Possible reasons will be discussed in relation to the structural properties of the electrodes. [1] Schnaid, Beckord, Engstfeld, Klein, Brimaud, Behm, PCCP 19 (2017) 4166

O 13.7 Mon 16:30 H16

The Effect of DFT Functionals on First-principles Estimates of the Free Energy Barrier of Water Deprotonation on TiO_2(110) — •Ahmad Agung, Thomas Stecher, Karsten Reuter, and Harald Oberhofer — Technische Universität München

Water splitting on TiO_2 is an important model reaction for photoelectrocatalytic processes in general. Recently, we calculated the kinetic barrier of the first deprotonation step on the rutile $TiO_2(110)$ surface based on ab-initio molecular dynamics (AIMD) and utilizing QM-MM embedding, explicit solvation, and the HSE06 hybrid functional.[1] However, the high computational cost of hybrid DFT and the size of the system render such an approach infeasible e.g. for possible catalyst screening studies. In our contribution, we therefore investigate a different approach based on semi-local DFT dynamics and a statistical re-weighting of snapshots with HSE06. We show that, although semi-local DFT by itself would give qualitatively wrong results, the re-weighting procedure restores the correct shape of the free energy profile along the reaction coordinate. We discuss the reasons for the failure of semi-local DFT and highlight remaining sources of error in the re-weighting procedure, leading to still present over-estimation of the free energy barrier height. This work is an important step towards a computationally feasible simulation protocol for free energy barriers in photo-electrocatalytic processes.

[1] T. Stecher, K. Reuter and H. Oberhofer, Phys. Rev. Lett. 117, 276001 (2016).

O 13.8 Mon 16:45 H16

Hydration structures of brookite TiO_2 (210) before and after UV irradiation — •Lei Yang[1], Eero Holmstrom[2], Takeshi Fukuma[3], and Adam Foster[2] — [1]WPI Nano Life Science Institute, Kanazawa University, Kanazawa 920-1192, Japan — [2]COMP, School of Science, Aalto University, P.O. Box 11100, FI-00076 Aalto, Finland — [3]Division of Electrical Engineering and Computer Science, Kanazawa University, Kanazawa 920-1192, Japan

TiO_2/H_2O interface has attracted wide attention due to the photocatalytic capabilities of this system. While rutile and anatase have been intensively researched, the brookite phase remains to be much less explored, despite its significant potential applications in CO_2 reduction and water splitting. Targeting these photocatalytic applications, we carried out *ab initio* molecular dynamics (AIMD) simulations and atomic force microscopy (AFM) as well as attenuated total internal reflection (ATR-IR) spectroscopy measurements to elucidate the hydration structures of brookite (210) surface before and after ultraviolet irradiation. We show the surface to feature a higher hydrophilicity and the interface to present a different topography after irradiation in our experiments. Simulations were performed to provide a molecular-level explanation for the topographic difference between the hydration structures of surfaces with different hydrophilicities on the basis of hydrogen bonding. The difference in vibrational properties is predicted by AIMD as well, which needs to be further validated by ATR-IR measurements.

O 13.9 Mon 17:00 H16

Interfacial water reorientation after UV irradiation of TiO2 — •Shumei Sun[1], Saman Hosseinpour[1], Simon Schlegel[1], Mischa Bonn[1], and Ellen Backus[1,2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Physical Chemistry, University of Vienna

Clean energy like hydrogen can be generated on TiO2 by photocatalytic water splitting with UV light, which was discovered more than 40 years ago. Since then, tremendous research efforts on TiO2 have been driven by the potential benefits for renewable energy. However, the mechanism behind photocatalysis is still unclear. Sum frequency vibrational spectroscopy as a surface sensitive technique allows us to probe the interface of TiO2/water. Here we use a femtosecond UV pulse as pump to excite TiO2. Subsequently, sum frequency vibrational spectroscopy is used as probe to monitor the response of water molecules to UV excitation of TiO2. Preliminary results show that electron and holes generated in the TiO2 by UV excitation recombine on a few hundred picoseconds timescale. Moreover, the interfacial structure seems to change on a sub-ps timescale, showing differences depending on the pH of the solution. Our results show that UV pump-SFG probe is a powerful tool to unravel the mechanism of a photon induced surface reaction.

O 13.10 Mon 17:15 H16

Functionalisation of catalyst and electrocatalyst surfaces by means of a femtosecond laser process — •Thomas Gimpel[1], Viktor Hoffmann[1], Matthias Koj[2], Andreas Gabler[1], Luise F. Hoffmann[1], Mia Börner[3], Anders Nilsson[3], Thomas Turek[2], and Wolfgang Schade[1,4] — [1]EST, Clausthal University of Technology, Goslar, Germany — [2]ICVT, Clausthal University of Technology, Clausthal-Zellerfeld, Germany — [3]Chemical Physics Division, Stockholm University, Sweden — [4]Fraunhofer Heinrich Hertz Institute, Goslar, Germany

Femtosecond laser ablation enables an increased surface and the formation of different structures up to the 100um range on many materials. Simultaneously, elements from the process environment are incorporated into the substrate surface. The additional elements may stem from a gaseous, liquid or a solid phase. Thus, with a single process step important material properties are tailored to some extent. We address especially the catalytic activity, the wettability, the heat transfer and fluid transport mechanisms. This contribution shows selected results from the electrochemical CO2 reduction reaction, a heterogeneous catalysis approach and in alkaline water electrolysis. This technique will help to develop tailored catalysts and electro catalysts beyond the mentioned applications.

O 14: Graphene II: Excitations and Nanoribbons (joint session O/TT)

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

O 14.1 Mon 15:00 H24

Altering the lattice dynamics of graphene by hot-electron injection — •Marcel Weinhold, Sangam Chatterjee, and Peter J. Klar — Institute of Experimental Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen

Graphene is discussed as material for next-generation (opto-)electronic devices. Among others, this is due to its exceptional properties including a large electron mobility, vast mechanical flexibility and durability, and its matchless linear and gap-less band structure. By combining graphene with metallic nanostructures that feature plasmonic characteristics its intrinsic properties can be tuned significantly. Those nanostructures lead to a near-field confinement of the incident light due to the excitation of localized surface plasmons (LSP). Further, LSPs decay non-radiatively into energy-rich electron-hole pairs. These 'hot-carriers' may be injected into the graphene and lead to a doping. However, plasmonic properties are very sensitive to geometry and dielectric environment. Therefore, single particle measurements are crucial for gaining further insights into the underlying physics. Here, we study the injection of hot-electrons in a model system, i.e., a single gold nanoparticle on a monolayer graphene substrate. We show that the injection of hot-electrons into graphene induces a quantifiable altering of graphene's phonon dispersion relation using specially resolved micro-Raman spectroscopy. In addition, we present an analysis procedure yielding further information on occurring temperature and strain distributions solely from the measured Raman shift maps.

O 14.2 Mon 15:15 H24

Single Spin Localization and Manipulation in Graphene Open-Shell Nanostructures — •Jingcheng Li[1], Sofia Sanz[2], Martina Corso[2,3], Deung Jang Choi[2,3,5], Diego Peña[4], Thomas Frederiksen[2,5], and Jose Ignacio Pascual[1,5] — [1]CIC nanoGUNE, 20018 Donostia-San Sebastián, Spain — [2]DIPC, 20018 Donostia-San Sebastián, Spai — [3]Centro de Física de Materiales (CSIC-UPV/EHU), 20018 Donostia-San Sebastián, Spain — [4]3CIQUS, Santiago de Compostela (Spain) — [5]Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Predictions state that graphene can spontaneously develop magnetism from the Coulomb repulsion of its π-electrons, but its experimental verification has been a challenge. Here, we report on the observation and manipulation of individual magnetic moments localized in graphene nanostructures on a Au(111) surface. Using scanning tunneling spectroscopy, we detected the presence of single electron spins localized around certain zigzag sites of the carbon backbone via the Kondo effect. Two near-by spins were found coupled into a singlet ground state, and the strength of their exchange interaction was measured via singlet-triplet inelastic tunnel electron excitations. Theoretical simulations demonstrate that electron correlations result in spin-polarized radical states with the experimentally observed spatial distributions. Hydrogen atoms bound to these radical sites quench their magnetic moment, permitting us to switch the spin of the nanostructure using the tip of the microscope.

O 14.3 Mon 15:30 H24

Molecular Spin Excitation by Electron Injection Through a Single Graphene Nanoribbon — •Niklas Friedrich[1], Jingcheng Li[1], Néstor Merino-Díez[1,2], Dimas G. de Oteyza[2], Diego Peña[3], David Jacob[4,5], and Nacho Pascual[1,5] — [1]CIC nanoGUNE, San Sebastian (Spain) — [2]DIPC, San Sebastian (Spain) — [3]CIQUS, Santiago de Compostela (Spain) — [4]Departamento de Física de Materiales, UPV/EHU, San Sebastian (Spain) — [5]Ikerbasque, Basque Foundation for Science, Bilbao (Spain)

Graphene nanoribbons (GNRs) and GNR-hybrids can be synthesized on metal surfaces with atomic precision using on surface synthesis techniques. Previously, we constructed a system in which chiral (3,1)-GNRs act as leads contacting a magnetic porphyrin molecule on a Au(111) substrate. Characterizing the porphyrin's magnetic properties by inelastic electron tunneling spectroscopy (IETS) we showed that the porphyrin's spin survives up to 4 contacting GNRs.

As a further step towards fully functional molecular devices, we now characterize the transport properties of linear GNR-porphyrin-GNR systems. We created a transport junction by contacting the system at a GNR end with the STM tip and lifting the molecular complex partially from the surface. We investigate the porphyrin's spin state via IETS by electrons cotunneling through the semiconducting GNR. In this transport configuration inelastic tunneling excites the Fe spin with excitation energies similar to the one measured by STS on surface. However, some molecular structures were found to lie in a mixed-valence state that vanished as the porphyrin was lifted from the metal.

O 14.4 Mon 15:45 H24

Segregated transport channels in sidewall nanoribbons — •Stephen Power[1,2,3], Johannes Aprojanz[4], Pantelis Bampoulis[5,6], Stephan Roche[1,7], Antti-Pekka Jauho[8], Harold Zandvliet[6], Alexei Zakharov[9], and Christoph Tegenkamp[4,5] — [1]ICN2, Bellaterra, Spain — [2]UAB, Bellaterra, Spain — [3]School of Physics, Trinity College Dublin, Ireland — [4]Institut für Physik, Technische Universität Chemnitz — [5]Institut für Festkörperphysik, Leibniz Universität Hannover — [6]MESA+Institute, University of Twente, The Netherlands — [7]ICREA, Barcelona, Spain — [8]CNG and DTU Nanotech, Denmark — [9]MAX IV Laboratory and Lund University, Sweden

Conductance quantization is a defining feature of electronic transport in quasi-one dimensional conductors. In the absence of a magnetic field, confinement results in a sequence of transverse sub-bands with an increasing number of nodes across the device width. Graphene nanoribbons grown on the sidewalls of SiC mesa structures have previously[1] been shown to present a 1D ballistic channel at the micron scale. New 2-point measurements reveal additional quantised channels at shorter probe separations[2]. Surprisingly, these channels are localised in different regions across the ribbon width. Here we demonstrate how this distribution of channels is consistent with a model accounting for both edge zigzag magnetism and asymmetric interfaces between the SiC and nanoribbon at each edge.

[1] J. Baringhaus et al, Nature 506 (2014) 349 [2] J. Aprojanz, S.R. Power et al, Nature Communications 9 (2018)4426

O 14.5 Mon 16:00 H24

Edge State Engineering of Graphene Nanoribbons — •Ping Yu — School of Physical Science and Technology, ShanghaiTech University

Zigzag edges of graphene nanoribbons are predicted to be spin-polarized and could have great potential for spintronics. The ability to precisely engineer the zigzag edge state is of crucial importance for realizing its full potential functionalities in device nanotechnology. Here, by combining scanning tunneling microscopy and atomic force microscopy, the zigzag edge states are found to get energy splitting upon fusing manganese phthalocyanine molecule with the short armchair graphene nanoribbon termini. Moreover, the edge state splitting can be reversibly switched by adsorption and desorption of atom hydrogen on the magnetic core of manganese phthalocyanine. The engineering mechanism is found to be due to the zigzag edge local doping level by the charge transfer process, which provides a new route to functionalize graphene-based molecular devices.

O 14.6 Mon 16:15 H24

How Structural Defects Affect the Mechanical and Electrical Properties of Single Molecular Wires — •Matthias Koch[1], Zhi Li[2], Christophe Nacci[1,3], Takashi Kumagai[1], Ignacio Franco[2], and Leonhard Grill[1,3] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]University of Rochester, Rochester, United States — [3]University of Graz, Graz, Austria

Graphene nanoribbons (GNRs) [1] are attractive candidates for molecular wires [2]; a key component in molecular nanotechnology. In addition to inheriting the supreme electromechanical properties of graphene [3], these narrow stripes offer a tunable band gap [4], which is crucial for electronic applications. Although many studies on molecular wires exist, the role of defects in the chemical structure has not been investigated. Here, we show how individual defects affect the properties of single GNRs [5]. Scanning tunnelling and atomic force microscopy (STM/AFM) pulling experiments access their electrical and mechanical properties simultaneously. We find, with the help of atomistic simulations, that defects substantially vary the molecule-substrate coupling and drastically increase the flexibility of the graphene nanoribbons while keeping their desirable electronic properties intact. Our study suggests that defected GNRs are suitable for molecular electronics that require flexible components, in contrast to rigid architectures.

[1] Cai, J. et al. Nature 466, 470 (2010) [2] Koch, M. et al. Nat. Nanotech. 7, 713 (2012) [3] Novoselov, K. S. et al. Nature 490, 192 (2012) [4] Han, M. Y. et al. Phys. Rev. Lett. 98, 206805 (2007) [5] Koch, M. et al. Phys. Rev. Lett. 121, 047701 (2018)

O 14.7 Mon 16:30 H24

Tailoring end states of graphene nanoribbons by magnetic dopants — •Tobias Preis, Sujoy Karan, Tobias Frank, Jaroslav Fabian, Ferdinand Evers, Dieter Weiss, Jonathan Eroms, and Jascha Repp — University of Regensburg, Faculty of Physics - Regensburg, Germany

Zig-zag edges of graphene are predicted to host spin-polarized electronic states and hold great promise for future spintronic device applications [1]. With the help of scanning tunneling microscopy (STM), we investigated the short zig-zag edges of bottom-up synthesized armchair graphene nanoribbons (GNRs), which were fabricated according to the recipe of Cai et al. [2]. We deposited single Co atoms on the surface and positioned them with the help of the STM tip underneath the GNRs. dI/dV spectra taken at the adsorption positions of embedded Co atoms show the emergence of a Kondo-like peak, being distinctly different from any Kondo features of isolated Co adatoms on the Au(111) surface. The peak exhibits a peculiar dependence on the position with respect to the short GNR edge.

[1] K. Nakada et al., PRB 54, 24 (1996)

[2] J. Cai et al., Nature 466, 470 (2010)

O 14.8 Mon 16:45 H24

On-surface synthesis of chevron-like graphene nanoribbons — •Koen Houtsma, Mihaela Enache, Ida Delac Marion, Tuan Anh Pham, Van Bay Tran, and Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, Groningen, the Netherlands

Graphene nanoribbons (GNRs) are a novel material that has aroused much interest because of its excellent and tunable electronic properties. Using on-surface synthesis, GNRs can be produced with atomic precision. In our research, GNRs with chevron-like topology were created via Ullman-type coupling from the prochiral molecular precursor 6,12-dibromocrhysene on a Au(111) surface. The structural properties of these GNRs, also in dependence of post-deposition annealing temperature, were investigated using scanning tunneling microscopy [1]. With scanning tunneling spectroscopy, we additionally characterized their electronic properties.

[1] T.A. Pham et al., Small 13 (2017) 1603675.

O 14.9 Mon 17:00 H24

Bottom-up fabrication of porous carbon nanoribbons on metal surfaces — •Mirunalini Devarajulu, Martin Haller, Maximilian Ammon, Min-Ken Li, Shadi Sorayya, and Sabine Maier — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

On-surface synthesis is a versatile technique to fabricate graphene-based nanoribbons from the bottom-up with high precision. We demonstrated that one-dimensional carbon nanoribbons with periodic hexagonal nanopores can be fabricated via Ullmann-type reactions on Ag(111) in combination with dehydrogenation reactions and the preprogrammed isomerization of the conformationally flexible precursor.[1] Here, we unveil the reaction mechanism and the N-doping of the porous nanoribbons in a low-temperature scanning tunneling microscopy study. We show that the rotation of *m*-phenylene units is a powerful design tool to promote structural control in the synthesis of porous covalent organic nanostructures on different metal surfaces. We find that the fabrication of porous nanoribbons proceeds on different terminations of the silver surface. However, the N-doping via triazine moieties influences the conformational selectivity of the molecular precursor, which affects the nanoribbon formation.

[1] M. Ammon, T. Sander, S. Maier, JACS, 2017, 139 (37), 12976

O 14.10 Mon 17:15 H24

Chevron-based graphene nanoribbons and heterojunctions by direct contact printing — •Axel Enders[1], Jacob D Teeter[2], Paulo S Costa[2], Gang Li[2], and Alexander Sinitskii[2] — [1]Universität Bayreuth, Physikalisches Institut, 95440 Bayreuth — [2]University of Nebraska - Lincoln, Lincoln NE 68588, USA

Atomically precise graphene nanoribbons (GNRs) have been synthesized through a direct contact transfer (DCT) of molecular precursors on Au(111), followed by gradual annealing. This method provides an alternative to the conventional approach for the deposition of molecules on surfaces by sublimation and simplifies preparation of dense monolayer films of GNRs. We performed STM characterization of the precursors of chevron GNRs, and demonstrate that the assemblies of the intermediates of the GNR synthesis are stabilized by π - π interactions. DCT was then used to deposit a mixture of two structurally similar but visually distinct chevron-type molecular precursors. Annealing of the deposited mix resulted in heterojunctions composed of units of chevron GNRs (cGNRs) and new laterally extended chevron GNRs (eGNRs). The electronic properties of these GNRs across the heterojunctions were studied with scanning tunneling spectroscopy. The dI/dV maps show that the impact of heterojunctions as well as structural defects is highly local and usually stays within the corresponding GNR units even if they are bonded to structurally and electronically different neighbors. It is expected that this method of DCT is highly versatile and allows to combine other chevron-type GNRs as well, such as nitrogen-doped cGNRs, into a variety of new GNR heterojunctions.

O 14.11 Mon 17:30 H24

Expitaxially grown twisted bilayer graphene on SiC(0001) — •You-Ron Lin[1,2], Nafiseh Samiseresht[1,2], Markus Franke[1,2], Shayan Parhizkar[1,2], François C. Bocquet[1,2], F. Stefan Tautz[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, 52425 Jülich, Germany

Layer by layer stacking of 2D-materials such as graphene, hexagonal boron nitride (hBN) and transition metal dichalcogenides (TMDCs) has been widely investigated developing a field on its own [1]. It has been shown that apart from the material used for stacking, the twist angle between two layers also has an immense effect on the band structure of the stack [2]. We report a reproducible method for large scale epitaxial growth of graphene bilayers utilizing the precursor molecule borazine. The existence of both graphene layers is confirmed by angular-resolved photoemission spectroscopy (ARPES). Spot-profile analysis low electron energy diffraction (SPA-LEED) has been used to determine a twist of $30 \pm 0.46°$.
[1] A. K. Geim *et al.*, *Nature*, **499**, 419, 2013.
[2] Y. Cao *et al.*, *Nature*, **556**, 43, 2018.

O 14.12 Mon 17:45 H24

Dielectric engineering in twisted bilayer graphene — •Jose Pizarro[1], Malte Rösner[2], Ronny Thomale[3], and Tim Wehling[1] — [1]Universität Bremen — [2]University of Southern California — [3]Universität Würzburg

Twisted bilayer graphene (TBG) has appeared as a tunable testing ground to investigate the conspiracy of electronic interactions, band structure, and lattice degrees of freedom to yield exotic quantum many-body ground states in a two-dimensional semiconductor framework. While the impact of external parameters such as doping or magnetic field can be conveniently modified and analyzed, the lack of open accessiblity of the quasi-2D electron gas combined with its intricate internal properties pose a challenging task to characterize the quintessential nature of the different insulating and superconducting states found in transport experiments. We analyze the possible role of the dielectric environment for TBG on the internal electronic interaction profile, which could be conveniently adjusted in experiment, e.g. by varying the capping layer composition and thickness. We find that this allows to significantly modify the internal interaction strength. In doing so, we propose the experimental tailoring of the dielectric environment as a promising pursuit to provide further evidence for resolving the hidden nature of quantum many-body states in TBG.

O 15: Metal Substrates II: Adsorption and Reactivity

Time: Monday 15:00–17:30 Location: Kunsthalle

O 15.1 Mon 15:00 Kunsthalle

Photon-Induced Processes at the Bromobenzene/Cu(111) interface — •John Thomas[1], Ishita Kemeny[1,2], Cord Bertram[1,3], Manuel Ligges[1], Karina Morgenstern[3], and Uwe Bovensiepen[1] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Stanford PULSE Institute, SLAC National Accelerator Laboratory — [3]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum

Bromine-substituted organic molecules are extensively used as precursors in on-surface synthesis where the molecules are activated through thermal dissociation. Hence, these synthesis processes are limited by the desorption temperature of the molecules of interest. If the desorption temperature is in the range of the dissociation temperature, photoinduced dissociation is an attractive alternative to activate these precursors. We present a systematic study of photo-induced processes in bromobenzene on Cu(111) from sub-monolayer to multilayer coverages and address structure and dissociation dynamics. Scanning tunneling microscopy delivers structural information in the regime below 0.5 monolayers where the molecules adsorb parallel to the surface. We observe the decomposition of molecular clusters and dissociation of molecules under ultraviolet photon irradiation at temperatures below 11 K. Using two-photon photoemission spectroscopy we monitor the activation of molecules through the work function change upon photo excitation and identify coverage-dependent electron attachment and dissociation processes.

This work is supported by the DFG through the cluster of Excellence RESOLV (EXC 2033).

O 15.2 Mon 15:15 Kunsthalle

Inducing the Controlled Rotation of Single o-MeO-DMBI Molecules Anchored to Au(111) — •Frank Eisenhut[1,2], Jörg Meyer[1,2], Tim Kühne[1,2], Jorge Monsalve[1,2], Justus Krüger[1,2], Robin Ohmann[1,2], Gianaurelio Cuniberti[1,2,3], and Francesca Moresco[1,2] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

A key step towards building single molecule machines is to control the rotation of molecules and nanostructures step by step on a surface. Here, we used the tunneling electrons coming from the tip of a scanning tunneling microscope to achieve the controlled directed rotation of complex o-MeO-DMBI molecules. We studied the adsorption of single o-MeO-DMBI molecules on Au(111) by scanning tunneling microscopy at low temperature and observed by lateral manipulation experiments that the molecules chemisorb on the surface and are anchored on Au(111) with an oxygen-gold bond via their methoxy group. Driven by inelastic tunneling electrons, o-MeO-DMBI molecules can controllably rotate, stepwise and unidirectional, either clockwise or counterclockwise depending on their enantiomeric form. Furthermore, we investigated the temperature-induced rotation of the molecules.

O 15.3 Mon 15:30 Kunsthalle

Following the products of a single intramolecular bond dissociation on surface — •Donato Civita, Grant James Simpson, and Leonhard Grill — Department of Physical Chemistry, University of Graz, Austria

Manipulation of molecules adsorbed at surfaces is very appealing to control and understand fundamental chemical processes. Chemical reactions can be triggered in single molecules by using a scanning tunneling microscope (STM). Specifically, chemical bonds within molecules can be cleaved [1], the resulting fragments can be pulled across the surface by lateral manipulation with the STM tip and even new bonds can be formed [2]. In this work, we study the dissociation of a single Br atom from a dibromoterfluorene (DBTF) molecule adsorbed on a Ag(111) surface. Experiments were done by applying voltage pulses with the STM tip on a single molecule at low temperatures (7 K). By imaging the single molecule before and after such a manipulation and, in addition, studying the current signal during the voltage pulse, we obtain insight into the process. Many dissociation experiments were recorded for different molecular isomers and different lateral locations of the voltage pulse over the molecule. A statistical analysis of the results reveals details about the dynamics of the dissociation, in particular the fate of the reaction products.

[1] B. C. Stipe, M. A. Rezaei, W. Ho, S. Gao, M. Persson, and B. I. Lundqvist, Phys. Rev. Lett. 78, 4410 (1997)

[2] K. Anggara, L. Leung, M. J. Timm, Z. Hu and J. C. Polanyi, Science Advances, EAAU2821 (2018)

O 15.4 Mon 15:45 Kunsthalle

Surface Chemical Bond of Alternant and Non-Alternant Aromatic Molecules: Influence of the Metal Surface — •Benedikt P. Klein[1], Lukas Ruppenthal[1], Markus Franke[2], Stefan R. Kachel[1], François C. Bocquet[2], Ralf Tonner[1], Christian Kumpf[2], Reinhard J. Maurer[3], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [3]Department of Chemistry, University of Warwick, United Kingdom

Metal/organic interfaces have a large impact on the performance of organic-electronic devices. The understanding of their chemical, electronic and geometric structure is therefore of great importance. Up to now, aromatic systems with alternant topology, such as pentacene, have been studied almost exclusively. To adress this neglect of the non-alternant topology, we investigated the adsorption of the non-alternant molecule azulene and its alternant counterpart naphthalene on the (111) surfaces of Cu, Ag and Pt, using a variety of methods including NEXAFS, PES, TPD, and NIXSW. To provide detailed insight into the surface chemical bond, we used complementary periodic DFT calculations including the deconvolution of DOS and NEXAFS simulations in the molecular orbital contributions. Our results show that the non-alternant molecule binds slightly stronger on Ag, where both molecules are physisorbed, and on Pt, where both are chemisorbed. On the Cu surface the difference is largest with the non-alternant molecule chemisorbed in contrast to the physisorbed alternant molecule.

O 15.5 Mon 16:00 Kunsthalle

Properties of Adsorbed Solvent Molecules: Adsorption Strength and Structure of $CDCl_3$ on Ag(111) — •Marvin Quack and Karina Morgenstern — Chair of Physical Chemistry I, Ruhr-University of Bochum, Germany

Characterizing the adsorption processes of solvent molecules on metal surfaces and the fundamental understanding of surface-adsorbate interactions play an important role, as for example in electrochemical cells or solid state catalysts. In order to understand the process of adsorption of solvent molecules, we investigated chloroform ($CDCl_3$) supported on a Ag(111) single crystal surface by means of temperature programmed desorption (TPD) and low-temperature scanning tunneling microscopy (LT-STM) in ultra high vacuum. The TPD spectra reveal the desorption of molecular chloroform below 180 K, indicating a physisorbed species. The STM results show the formation of a (2x2) superstructure at coverages lower than 1 ML of $CDCl_3$. At higher coverage, we observe the growth of 1D-crystallites in the second layer following the high symmetry directions of the substrate. Further STM results and a model for the adsorption will be presented in this talk.

O 15.6 Mon 16:15 Kunsthalle

Kinetic control of reaction products in porphine oligomerization on Au(111) — Knud Seufert[1,3], •Simon Jaekel[1], Leonhard Grill[1], Fiona McBride[2], Bareld Wit[2], Shamsal Haq[2], Rasmita Raval[2], Paolo Poli[2], and Mats Persson[2] — [1]Institut für Chemie, Universität Graz — [2]Dept. of Chemistry, University of Liverpool — [3]Fakultät für Physik, TU München

Nanostructures built from porphyrins have shown much promise in diverse applications such as light harvesting, optoelectronics, gas sensing and molecular electronics [1,2,3]. Investigating these nanostructures on metallic surfaces allows investigations of the electronic properties of individual nanostructures [3]. It has been shown that such nanostructures can be synthesized on surfaces through homocoupling of porphyrin molecules at the macrocycle[4,5]. The resulting oligomers are of particular interest as they are fully conjugated and the reaction leaves no side products on the surface.

Here, we report scanning tunneling microscopy results for porphine coupling on Au(111). The binding motifs of the reaction products are shown to be not only determined by energetic stability, but also by the reaction kinetics. Therefore, the final structure and hence electronic properties of the oligomers can be tuned via different reaction pathways while using the same monomers.

[1]Lin et al. Science 1994, 264, 1105 [2]Nguyen et al. Phys. Rev. B 2008, 77, 195307 [3] Kuang et al. J. Am. Chem. Soc 2016, 138, 11140 [4] Wiengarten et al. J. Am. Chem. Soc. 2014, 136, 9346 [5]Xiang et al ACS Nano 2018, 12, 1203

O 15.7 Mon 16:30 Kunsthalle

Frequency modulation atomic force microscopy and scanning tunneling microscopy study of CO on Pt(111) — •Oliver Gretz, Franz J. Giessibl, and Alfred J. Weymouth — Universität Regensburg, Regensburg, Deutschland

Small molecules, like CO, have a higher binding energy to platinum than to other metals like copper. When comparing CO on Pt(111) to CO on Cu(111), the frustrated translational mode is 2 meV (about 50%) higher and individual CO molecules appear in low-bias STM images as protrusions instead of as depressions. In this talk we present our AFM/STM studies of CO on Pt(111). Previously, CO on Cu(111) has been used to image the apex of an AFM tip (CO-Front atom Identification - COFI). As the lateral stiffness of adsorbed CO scales by the square of the energy of the frustrated translational mode, we expect less abberations due to CO bending than on Cu(111). We performed COFI measurements with CO on Pt(111). In addition, we performed manipulation experiments and measured the lateral force to move a CO molecule from one adsorption site to another.

O 15.8 Mon 16:45 Kunsthalle

Energy Dissipation Mechanisms for CO+O Association on Ru(0001) on Femtosecond Timeframes — •Manuel J. Kolb[1,2,3], Frank Abild-Pedersen[1,2], and Lars G.M. Pettersson[3] — [1]SLAC National Laboratory, Stanford, USA — [2]Stanford University, Stanford, USA — [3]Alba Nova, Stockholm University, Stockholm, Sweden

Recent work in our group[1] on CO+O association taking place on the Ru(0001) surface revealed that the reaction pathway exhibits two independent transition states, with the first of these being rate-determining. However, in contrast to conventional expectations, a significant population was observed in the low-energy region spanned by the two transition states. Here, we present a theoretical investigation into possible energy dissipation mechanisms which account for this increased occupation: Firstly, the energy loss due to electronic friction along the pathway. Secondly, we investigate the energy transfer to and from the individual vibrational degrees of freedom of the CO-O complex to the substrate and its influence on the individual reaction energy barriers.

[1]Henrik Öström et al., Science, 2015, 347, 6225, pp 978-982

O 15.9 Mon 17:00 Kunsthalle

The role of the surface in the atomic oxidation of supported Coronene films — Jürgen Weippert, Vincent Gewiese, Seyithan Ulas, Dmitry Strelnikov, •Artur Böttcher, and Manfred M. Kappes — Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

Atomic oxidation of Coronene films grown on HOPG results in the formation of various surface species, $C_mH_nO_k$, which subsequently can be desorbed as intact nm-sized graphene oxides, nano-GOs. Coronene films were grown at room temperature by low-energy cluster ion beam deposition (LECBD, $C_{24}H_{12}^+$) and oxidized by exposing them to a beam of near-thermal atomic oxygen. The XPS-based analysis indicated that the oxidation of the $C_{24}H_{12}$ films proceeds predominantly via the formation of epoxides, ethers, and quinones. The mass spectrometric analysis of the subliming species revealed a strong dependency on the film thickness. The sublimation of thick oxidized Coronene films proceeds predominantly via the emission of rim-epoxides $C_{24}H_{12}O_n$ ($n \leq 7$) [1]. The sublimation from oxidized thin films, $\Theta \leq 2$, exhibits lactones $C_{23}H_{10}O_2$ and dilactones $C_{22}H_8O_4$. The sublimation from Coronene monolayers deposited on a pre-oxidized basal plane is also dominated by the aforementioned oxides.

[1] J. Weippert, et al. JPC C 2018, DOI: 10.1021/acs.jpcc.8b01655

O 15.10 Mon 17:15 Kunsthalle

Solvent Induced Growth Polymorphs of 1,3-Dithia Derivatives of Ferrocene on HOPG — •Thiruvancheril G. Gopakumar[1], Prithwidip Saha[1], Vinithra Gurunarayanan[1], Vladimir V. Korolkov[2], Prema G. Vasudev[3], Ramesh Ramapanicker[1], and Peter H. Beton[2] — [1]Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India — [2]School of Physics and Astronomy, The University of Nottingham, Nottingham NG7 2RD, United Kingdom — [3]Molecular and Structural Biology Department, CSIR-Central Institute of Medicinal & Aromatic Plants, Lucknow UP-226015, India

Ferrocene (Fc) and its derivatives have attracted interest in electronic applications[1] due to its tunable of electronic properties. In this work we have studies the microscopic structure of ultra-thin films of two 1,3-dithia derivatives of Ferrocene (Fcs) on the basal plane of highly oriented pyrolytic graphite (HOPG) using AFM and STM at ambient conditions. Films are prepared by drop-casting Fcs dissolved in different solvents. Upon deposition of Fcs from methanol and DCM, two types of molecular growth polymorphs are observed. When Fcs are deposited from ethanol, acetone, DMF and toluene, one of the growth polymorphs is exclusively observed. The formation of growth polymorphs are understood using the boiling point of solvents and the solubility of Fcs in solvents.[2] Solvents with high boiling point prompts the formation of energetically favorable growth.

[1] N.Nerngchamnong et al. Nat. Nanotechnol. 2013, 8, 113. [2] P. Saha et al. J. Phys. Chem. C, 2018, 122, 19067.

O 16: Mechanically Controlled Electrical Conductivity of Oxides (joint session MM/CPP/O)

Sessions: SYCO II and III

Time: Monday 15:45–18:30 Location: H46

Topical Talk O 16.1 Mon 15:45 H46

Probing the properties of dislocations in $SrTiO_3$ through transient transport measurements — •Roger De Souza — Institute of Physical Chemistry, RWTH Aachen University, 52056 Aachen, Germany

There is renewed interest in the interaction between oxygen vacancies and dislocations in the perovskite oxide $SrTiO_3$, driven by the material's possible application in devices for all-oxide electronics and for resistive switching. In my talk, I will demonstrate how transient transport experiments — comprising $^{18}O/^{16}O$ isotope exchanges and Secondary Ion Mass Spectrometry (SIMS) analysis — can be used to obtain a deeper understanding of this interaction. Having first introduced the thermodynamics of space-charge formation at extended defects, I will focus on describing experiments and simulations on various geometries: annealed single crystals, bicrystals, and polished single crystals. Finally, I will discuss how these studies allow us to arrive at a consistent description of point-defect behaviour at dislocations in $SrTiO_3$.

O 16.2 Mon 16:15 H46

Characterization of Fe:STO thin films prepared by pulsed laser deposition — •Maximilian Morgenbesser, Stefanie Taibl, Markus Kubicek, Alexander Viernstein, Christopher Herzig, Andreas Limbeck, and Jürgen Fleig — TU Wien, Wien, Österreich

The perovskite-type oxide SrTiO3 (STO) is one of the best investigated materials in solid state ionics and commonly used as a model material in solid state ionics. The defect model of bulk SrTiO3 is well understood and the conductivity of bulk samples can be tailored by acceptor or donor doping, e.g. with Fe3+ or Nb5+ on the Ti4+ site. However, other aspects of SrTiO3 have not been understood so far, for example the the influence of factors such as stoichiometry and strain on the conductivity which is investigated in this study.

Two different kinds of 2 % Fe-doped thin films were deposited by pulsed laser deposition (PLD). Thin films deposited from stoichiometric targets exhibit a low, intrinsic conductivity. In addition, targets with Sr overstoichiometry were used and the conductivity could be increased by four orders of magnitude. The thin films are compared to each other in regard to the structure and stoichiometry. Structural differences could be found by x-ray diffraction measures, revealing a difference in lattice parameters. The chemical composition was analyzed by means of inductively coupled plasma optical emission spectroscopy (ICP-OES) and differences in the A/B ratios could be found. A model linking the conductivity to the stoichiometry of the thin films is presented, highlighting the possible impact of cation vacancies and antisite defects on the electrical conductivity of Fe:SrTiO3.

O 16.3 Mon 16:30 H46

Generation of controlled dislocation structures in SrTiO3 and TiO2 for elucidating dislocation impact on electrical properties. — •Lukas Porz, Till Frömling, and Jürgen Rödel — Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Germany

Dislocations have been understood to alter numerous functional properties of ceramic materials, such as conductivity[Whitworth 1975]. Recently, modification of functional properties of oxide materials by dislocations receives much attention due to their various potentials for application[Szot 2018]. Especially the complex dislocation structure of naturally occurring dislocations makes investigations of dislocation effects difficult. Thus, disentangling the different effects of dislocations requires an ordered structure of the dislocations. So far ordered structures were primarily fabricated in bi-crystal interfaces which are often not comparable to natural dislocation arrangements.

We present a route to control the arrangement of the dislocations locally. Different slip systems can be individually introduced and an arrangement of all dislocations lying in the same set of slip planes was achieved. With identical line vectors, the dislocations connect two surfaces of a bulk sample which was shown by dark field x-ray microscopy. This well-arranged and well-understood structure of dislocations is a pre-requisite for unambiguous interpretations of detailed experiments on functional properties. The value of a controlled arrangement of dislocations is demonstrated by conductivity data along dislocation lines and across slip bands in comparison to a dislocation free reference.

45 min. break

O 16.4 Mon 17:30 H46

Atomic and electronic structure of wurtzite ZnO(0001) inversion domain boundaries — •Jochen Rohrer and Karsten Albe — FG Materialmodellierung, FB Material- und Geowissenschaften, Technische Universität Darmstadt

In a recent work [1], variations of the conductivity of ZnO bicrystal samples with $(0001)||(0001)$ and $(000\bar{1})|(000\bar{1})$ orientations (inversion domain boundaries, IDB) due to the modulation of the potential barrier height at the IDB with respect to strain [2] has been demonstrated. In order to establish a more profound understanding of this behavior, a detailed characterization of the atomic structure and electronic properties of such IDBs by means of first-principles methods will be valuable. However, despite the structural and chemical variability of this system, only a few atomistic models have been in studied to date [3].

In this work we comprehensively study ZnO$\{0001\}$ IDBs by means of density functional theory calculations. In particular, we construct a variety of structurally and chemically different phase-pure models and identify their thermodynamic stability within the allowed range of the O chemical potential. For stable models we investigate electronic properties and their response to strain. Finally we also study the role of various dopants, commonly added in experimental bicrystal samples.

[1] P. Keil *et al.*, *Adv. Mater.* **30**, 1705573 (2018). [2] D. R. Clarke, *J. Am. Ceram. Soc.* **82**, 485 (1999). [3] S. Li *et al.*, *Phys. Status Solidi B* **255**, 1700429 (2017).

O 16.5 Mon 17:45 H46

Impact of internal electric field on the grain boundary barrier height of ZnO — •Bai-Xiang Xu, Ziqi Zhou, and Till Frömling — Institute of Materials Science, TU Darmstadt

Polycrystalline ZnO ceramics with grain boundary potential barriers are important materials for surge arresters due to their non-linear current-voltage behavior, and have potential application in advanced devices. Different grain boundary barrier height models have been developed by considering the direct piezoelectric effect. However, the piezoelectric charge should not only result from the direct piezoelectric effect, but also from the inverse piezoelectric effect, which refers to the mechanical response of the material by the electric field. Due to the charges at the grain boundary, strong internal electric field can be expected, and it leads to strain change through the inverse piezoelectric effect. This strain further modifies the polarization and thus leads to additional piezoelectric charges at the grain boundary and in the depletion layer. Thus, this should also be taken into account self-consistently. For this purpose we employ both analytical model and finite-element numerical simulation to reveal the impact of internal electric field on the GB barrier height and its stress sensitivity. Results show that the piezoelectric charge induced by the internal field tends to adjust the grain boundary charge and lowers the barrier height. Furthermore, the barrier height becomes less sensitive to mechanical stress and applied voltage if the influence of the internal field is taken into account. The extended model with the inverse piezoelectric effect of the internal field allows to further elucidate their piezotronic response.

O 16.6 Mon 18:00 H46

Influence of cation order and strain on Na diffusion in $Na_3Zr_2Si_2PO_{12}$: A computational study — •Lisette Haarmann and Karsten Albe — Technische Universität Darmstadt, Otto-Berndt-Str. 3 64287 Darmstadt

$Na_3Zr_2Si_2PO_{12}$ is a solid electrolyte which is part of the Na super ionic conductor (NASICON) family. Experimentally, only Si/P lattice positions can be determined, but not the distribution of P on these sites[1]. This distribution, however, plays a crucial role for the Na diffusion. A systematic study of different cation orders is conducted using Molecular Dynamics (MD) simulations. Due to the strong correlation of diffusion in this material, the calculation of D_σ is necessary to obtain the ionic conductivity from the Nernst-Einstein equation[2]. By calculating D_σ and the tracer diffusion coefficient D_{tr}, Haven ratios are determined. Additionally, a jump rate model was developed, which allows investigation of correlation between individual jumps.

Moreover, it has been reported that doping can strongly increase the diffusivity of Na in NASICON materials[3]. In many cases, this is attributed to enlarged bottlenecks of diffusion. These doping elements, however, do not only contract or dilate the lattice structure but alter the chemical environment of the Na ions as well. In an effort to study purely the effect of mechanical deformation, the strain dependence of D_{tr} and the activation energy E_A is investigated.

[1] Boilot, J.P., *et. al.*, Journal of Solid State Chemistry **73**, (1988)
[2] Murch, G., Solid State Ionics **7**, (1982)
[3] Guin, M., Tietz, F., Journal of Power Sources **273**, (2015)

O 16.7 Mon 18:15 H46

The impact of mechanical stresses on the ionic conductivity of nanoparticles — •Peter Stein[1], Bai-Xiang Xu[1], and Karsten Albe[2] — [1]TU Darmstadt, FB 11, FG Mechanik funktionaler Materialien — [2]TU Darmstadt, FB 11, FG Materialmodellierung

Nanostructured electrodes have found wide application in electrochemical systems, for instance for lithium-ion batteries. This is due to their featuring short diffusion paths and large surface areas, allowing for comparatively fast surface reactions and transport within the slender bulk material. At this length-scale, surface stresses acting on the electrode surface induce a (non-uniform) pressure within the material, providing mechanical stabilization. As a result, nanostructured electrodes exhibit high reversible capacities and stable cycling behavior [1] as well as a higher robustness against mechanical degradation [2]. However, the surface-induced pressure field also affects the electrochemical behavior of the particle, modifying, among other things, surface reaction rates and ionic mobility.

In this contribution, we discuss the interaction of mechanical stresses with the electrochemical behavior of nanostructured electrode particles. We thereby consider ideal analytical shapes, faceted nanoparticles, and regular nanostructures such as inverse opal electrodes. We further demonstrate the impact of surface-stress-induced mechanical fields on defect thermodynamics and kinetics, chemical reactions, and phase transformations.

[1] N. Zhao et al., Pure Appl. Chem. 80:2283-2295, 2008. [2] C.K. Chan et al., Nat. Nanotechnol. 3:31-35, 2008.

O 17: Poster Monday: 2D Materials

Time: Monday 17:45–20:00 Location: Poster F

O 17.1 Mon 17:45 Poster F

Local charge transport in graphene devices mapped using Kelvin probe force microscopy — •Sayanti Samaddar[1], Kevin Janssen[1], Kai Sotthewes[2], Zhenxing Wang[3], Daniel Neumaier[3], Marcus Liebmann[1], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Otto-Blumenthal-Str., 52074 Aachen, Germany — [2]Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500AE Enschede, The Netherlands — [3]Advanced Microelectronic Center Aachen (AMICA), AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen

Graphene based field effect transistors (FETs) and diodes were investigated using KPFM in combination with transport. Imaging FETs, at different source to drain voltages, enables a mapping of local voltage drops occurring at various surface perturbations like defects, impurities, and wrinkles. In the regions between graphene wrinkles and the contacts, a strong enhancement of the potential gradients along the direction of current flow is observed. The response of these local voltage drops to a global back-gate is also investigated. In the second part, diodes comprised of titanium - titanium oxide - graphene heterostructures are studied, where gate voltages induce variations in the graphene work-function resulting in their superior asymmetry in comparison to metal-insulator-metal diodes [1]. We observe significant doping disorder ~ 50 meV on the graphene, which systematically decrease as the diode is tuned from the off state to the on state.

[1] M. Shaygan et al., Nanoscale 9, 11944 (2017)

O 17.2 Mon 17:45 Poster F

Electronic transport in Gold-contacted graphene on Germanium — •Simeon Bode[1], Anna Sinterhauf[1], Manuel Auge[2], Mindaugas Lukosius[3], Christian Wenger[3], Gunther Lippert[3], Hans Christian Hofsäss[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany — [2]II. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany — [3]IHP, 15236 Frankfurt (Oder), Germany

The successful growth of large-scale graphene on Ge/Si(001) is a large step towards the integration of graphene into silicon technologies [1]. However, since the exploration of graphene-based devices necessarily includes graphene-metal contacts, the quality of these contacts crucially limits the performance of the device. Therefore, an in-depth investigation of metal contacts on graphene on Ge/Si(001) is required. In this study, we use Kelvin probe force microscopy with an additionally applied electric field across the sample to analyze the local electrostatic potential of Gold-contacted graphene on Ge/Si(001). We find an exceptional sheet reistance for the graphene layer, whereas the electronic transport is significantly hindered close to the contacts due to the formation of a transition region. Additionally, element analysis using Rutherford backscattering reveals that the Au contact is not homogeneous; instead, an AuGe alloy forms in the contact region with a Gold Germanium ratio of approximately 50:50. This work is financially supported by the DFG through the SFB1073.

[1] Lukosius et al., ACS Appl. Mater. Interfaces 8, 33786-33793, 2016

O 17.3 Mon 17:45 Poster F

Atomistic simulations of chemical graphene exfoliation and carbon nanotube synthesis and of extended defects in bilayer graphene — •Florian Wullschläger, Robert Maidl, Konstantin Weber, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Results of three recent molecular dynamics (MD) and density functional theory (DFT) studies on graphene and carbon nanotubes (CNTs) will be presented. Reductive graphite intercalation with alkali metals and subsequent dispersion in tetrahydrofuran (THF) leads to an almost complete exfoliation of graphite into graphene monolayers. The properties of the exfoliation product in liquid THF have been investigated by force-field MD simulations and first insights into role of different alkali metals in the exfoliation process will be given. Second, with force field and DFT calculations we identified the crucial reaction step in the on-surface synthesis of CNTs with controllable and defined chirality by rolling-up appropriate precursor molecules via cyclodehydrogenation reactions. Finally, by using a specifically adapted registry-dependent interlayer potential we show that the properties of dislocations in quasi-2D crystals, i.e. bilayer graphene, differ significantly from their 3D counterparts [1]. In addition to an in-depth structural characterization of 2D dislocations, first results on the dislocation structure in twisted graphene bilayers will be given.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spiecker, Nature **505** (2014) 533.

O 17.4 Mon 17:45 Poster F

Local Manipulation and Exfoliation of Graphene from an HOPG Surface using a Scanning Tunneling Microscope — •Suchetana Sarkar[1], Christoph Dobner[1], Andreas Raabgrund[2], and Axel Enders[1] — [1]Universitaet Bayreuth, Bayreuth,Deutschland — [2]Friedrich-Alexander-Universitaet Erlangen-Nürnberg, Erlangen, Deutschland

Among the several methods in which graphene can be fabricated, the manipulation of graphitic surfaces has long been of interest. Here, we demonstrate a reliable method of forming Single Layer Graphene (SLG) and Few Layer Graphene (FLG) through the local electro-exfoliation of the top layers of HOPG. Using an ambient scanning tunneling microscope (STM), we create triangular graphene flakes by scanning perpendicular to a step edge which can then be peeled back via a voltage ramp, thereby detaching it from the substrate.These triangular flakes are of interest as they behave like isolated graphene sheets and can therefore be studied to gain insights into the correlation between surface morphology and electronic properties and the possibility to tune local conductance by surface manipulation. Under certain conditions, the creation of graphene flakes near macroscopic defects and backfolding onto the HOPG terrace, led to the formation of Moiré patterns. By using 1,2,4-Trichlorobenzene to intercalate the layers of HOPG in solution, Moiré lattices as large as 200 nm were achieved. Subsequent STM studies show that these exhibit different lattice periodicites, from which we can determine precisely how the graphene layers are aligned.

O 17.5 Mon 17:45 Poster F

Transfer-Free, Highly Crystalline Graphene on Insulator for Novel Applications in Electronics — •Håkon Ivarssønn Røst[1], Justin W. Wells[1], Rajesh Kumar Chellappan[1], Anton Tadich[2], Zheshen Li[3], and Antonija Grubišić Čabo[4] — [1]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology (NTNU), N-7491 Trondheim, Norway — [2]Australian Synchrotron, 800 Blackburn Rd., Clayton, Victoria 3168, Australia — [3]Department of Physics and Astronomy, Ny Munkegade 120, 8000 Aarhus C, Denmark — [4]School of Physics & Astronomy, Monash University, Clayton, Victoria 3168, Australia

Problems associated with the preparation of high-quality and contamination-free graphene on semiconductor that does not heavily interact with its underlying substrate has so far hindered its large-scale integration in device structures. This study presents a method for growing graphene on silicon carbide (SiC) by means of various transition metal catalysts, with subsequent intercalation of silicon and oxygen under the graphene layers to form an electrically insulating dielectric layer. The interaction of thin metal films with thermally treated SiC mediates liberation of carbon, allowing the formation graphene on semiconductor at temperatures down to 600°C. Intercalation of silicon and oxygen then decouples the graphene from its substrate by forming an insulating silicon oxide layer. The result is highly crystalline top layers of free-standing graphene, where the thickness of the interfacial dielectric layer can be tuned by the amount of silicon that gets intercalated prior to the oxidation step.

O 17.6 Mon 17:45 Poster F

Simulating the scattering of a hydrogen atom from graphene using a high-dimensional neural network potential. — •Sebastian Wille[1,2], Marvin Kammler[2], Martín L. Paleico[3], Jörg Behler[3], Alec M. Wodtke[1,2], and Alexander Kandratsenka[2] — [1]Institute for Physical Chemistry, Georg-August University Göttingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany — [3]Theoretical Chemistry, Georg-August University Göttingen, Germany

To fully understand atom-surface interactions, the availability of an accurate full-dimensional potential energy surface (PES) is crucial. High-dimensional neural network potentials have been shown to provide very accurate PESs for a wide range of systems. We developed a neural network potential for H-atom at a graphene sheet by fitting to density functional theory data calculated on-the-fly in *ab initio* molecular dynamics simulations. Based on this potential, we studied the scattering under various incidence conditions (like angle, kinetic energy, temperature) and compared the results to experimental data.

O 17.7 Mon 17:45 Poster F

3d transition metal clusters on defected graphene — •Xin Chen, Yuhang Liu, and Biplab Sanyal — Department of Physics and Astronomy, Uppsala University, Box 516, 751 20 Uppsala, Sweden

Adsorbing transition metal atoms on defected graphene is reported as one of the best routines to introduce magnetism in graphene. In this contribution, based on a first principles Born-Oppenheimer molecular dynamics simulations, we investigated the self-assembled processes of transition metal hexamers X_6 (X = Cr, Mn, Fe) on graphene with mono-/divacancy defects and discussed the fundamental electronic and magnetic properties of the resulting X_6 clusters on graphene from density functional theory. Interestingly, the ground state of Cr_6 and Fe_6 hexamers on divacancy graphene shows a quite small energy difference between in-plane and out-of-plane magnetism, and it can be easily manipulated by an external electric field, which promises applications in electric field assisted magnetic recording and quantum computing. We have also obtained insights into the switching of the easy magnetic axes, which revealed that specific d orbital symmetries of the transition metal atoms trapped in the vacancy site play a dominating role.

O 17.8 Mon 17:45 Poster F

Graphene at its Van Hove singularity and beyond — •Philipp Rosenzweig[1], Hrag Karakachian[1], Dmitry Marchenko[2], Kathrin Müller[1], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, 12489 Berlin, Germany

By intercalating ytterbium atoms underneath the carbon buffer layer on SiC(0001) we induce strong n-type doping in the resulting graphene monolayer. The π-band system shifts down such that the Van Hove singularity connecting $\overline{\mathrm{K}}$ and $\overline{\mathrm{K}}'$ via $\overline{\mathrm{M}}$ reaches the Fermi level E_F. The Fermi surface thus undergoes a Lifshitz transition, consisting of a single giant pocket around $\overline{\Gamma}$ as opposed to two pockets centered at $\overline{\mathrm{K}}$ and $\overline{\mathrm{K}}'$ for moderately-doped graphene systems. In addition, severe hybridization is observed between the graphene π-bands and the Yb $4f$ core levels near E_F, which might induce considerable spin-orbit splitting of graphene's Dirac cone [Marchenko et al., Nat. Commun. **3,** 1232 (2012)]. We further show that the doping level can be enhanced by potassium adsorption at cryogenic temperatures whereas sequential annealing at elevated temperatures leads to a gradual decrease in carrier density. Thus, via precise tuning of the experimental parameters, coherent control of graphene's doping level in the vicinity of its Van Hove singularity is achieved and the Lifshitz transition is observed in situ. Our studies might contribute to the experimental realization of exotic ground states in highly-doped graphene such as chiral superconductivity [Nandkishore et al., Nat. Phys. **8,** 152 (2012)].

O 17.9 Mon 17:45 Poster F

Intercalation of gold between graphene and silicon carbide studied by PEEM and XPS — •Philipp Weinert, Richard Hönig, Peter Roese, Karim Shamout, Malte Schulte, Ulf Berges, and Carsten Westphal — Experimentelle Physik I, TU

Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

Due to its outstanding electronic and mechanical properties graphene is highly interesting for many applications, for example as a new material in transistor applications and to build microscale structures.

In this study, the intercalation of gold between graphene and the substrate silicon carbide is investigated. Other investigations have shown, that covalent bounds between the the silicon carbide and the first carbon layer are released by intercalation, which leads to quasi free standing graphene.

To achieve the intercalation, samples have been coated with thin gold-films of different thickness. Subsequently, the samples have been annealed to cause the intercalation. In different steps of the annealing process, photoemission electron microscopy (PEEM) had been carried out for structural and X-ray photoelectron spectroscopy (XPS) for chemical investigation. Furthermore, the intercalation of silver between graphene and silicon carbide has been studied by PEEM.

O 17.10 Mon 17:45 Poster F

Influence of Li implantation on the transport properties of graphite flakes — •Johannes Küpper, José Barzola-Quiquia, Pablo Esquinazi, and Jan Meijer — Felix-Bloch-Institut für Festkörperphysik Universität Leipzig

The influence of Li implantation into mesoscopic thin graphite samples on their electrical transport properties were studied as a function of temperature and applied magnetic field. The temperature dependence of the electrical resistance before and after implantation is well described using a semiconducting contribution from the crystals and an additional metallic-like contribution due to the interfaces between them in parallel. We observe that with an increase of implantation dose the temperature dependence of the resistance gets more semiconducting, the resistivity increases an the magnetoresistance decreases. Fast fourier analysis of the Shubnikov de Haas oscillations indicates that the virgen sample is dominated by one carrier type, whereas for the implanted samples we observe the emergence of a new carrier type. Berry phase analysis of the Shubnikov de Haas oscillations indicates that our sample has 2D type charge carriers. Finally, using magnetic force microscoopy we investigate the effect of Li implantation on the creation of magnetic structures in these samples.

O 18: Poster Monday: Nanostructures

Time: Monday 17:45–20:00 Location: Poster F

O 18.1 Mon 17:45 Poster F

Theoretical investigation of H adsorption at the Si(557)-Au surface — •Ferdinand Ziese, Kirs Holtgrewe, Christof Dues, and Simone Sanna — Justus-Liebig-Universität Giessen, Institut für Theoretische Physik Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Vicinal Si(111)-Au surfaces feature single or double atomic Au chains on each terrace of the stepped Si surface [1]. The metallic wires are electronically decoupled from the substrate and represent quasi 1D nanoobjects. In order to tune the wire metallicity, different atoms and molecules can be adsorbed on the system [2]. In this work, we investigate the adsorption atomic hydrogen at the Si(557)-Au surface within density functional theory. In a first step, the favorable adsorption site is determined as a function of the H coverage by means of potential energy surface calculations. While H adsorbs on the Si step edge on pristine surfaces, the favored site for the secondary H adsorption is on top of the so-called rest atom. Band structure calculations reveal that H acts as an electron donor, influencing the electronic states related to the adsorption sites. For an H coverage corresponding to two H atoms per (5x2) surface unit cell, we predict the formation of an electronic band gap at the Fermi energy and a metal-to-insulator transition.

[1] N. J. Crain et al., Phys. Rev. B 69, 125401 (2004)

[2] Z. Mamyev et al., Phys. Rev. Mat. 2, 066002 (2018)

O 18.2 Mon 17:45 Poster F

Theoretical investigation of the Au-induced Si(111) surface reconstruction — •Felix Bernhardt, Kris Holtgrewe, Christof Dues, and Simone Sanna — Justus-Liebig-Universität Giessen

The Au-induced reconstruction of the Si(111) surface is one of the most intensively investigated nanostructured systems. It features quasi one-dimensional (1D) chain structures, which are prototypical 1D metals on a 2D semiconducting surface. The debate on the structural model of the Au wires has been periodically reignited, with the theoretical models proposed by Erwin, Barke and Himpsel [1], Abukawa and Nishigaya [2], as well as Kwon and Kang [3], marking the cornerstones of a long investigation process. Although the Kwong-Kang model is currently accepted, there have been several attempts to refine the structure, e.g., by surface x-ray diffraction [4]. A structural modification has been proposed recently by the Wollschläger group in Osnabrück. In this work, we test different structural modifications proposed by the experiment within density functional theory. Thereby we analyze the bond lengths as well as the energetics of the relaxed structural models within different computational schemes. The calculations reveal that the proposed modifications do not lead to a new structural model, but rather relax to the Kwong-Kang structure. [1] S. C. Erwin et al., Phys. Rev. B 80, 155409 (2009) [2] Abukawa et al., Phys. Rev. Lett. 110, 036102 (2013) [3] S.-W. Kwon et al., Phys. Rev. Lett. 113, 086101 (2014) [4] T. Shirasawa et al., Phys. Rev. Lett. 113, 165501 (2014)

O 18.3 Mon 17:45 Poster F

First-principles investigation of the vibrational properties of rare-earth silicides on the Si(111) surface — •Vincent Maximilian Wettig, Kris Holtgrewe, Christof Dues, and Simone Sanna — Justus-Liebig-Universität Gießen, Gießen, Hessen

The investigation of the vibrational properties has recently become one of the most appealing tools for surface analysis. As Raman frequencies and selection rules are strongly related to the surface structure, they represent reliable criteria to identify, validate or rule out competing structural models [1].

In this work, we model from first principles the vibrational properties of rare-earth silicide monolayer structures deposited on Si(111) surfaces. As the resulting metal/semiconductor interface is characterized by an extraordinarily low Schottky-barrier height (0.3*0.4 eV on n-type substrates), the silicide nanostructures are both of technological and academic interest.

Employing previously proposed structural models based on the hexagonal DySi2 lattice [2], we demonstrate the existence of surface localized phonon modes of different symmetry in the frequency range between 25 and 500 cm-1 for the investigated dysprosium and terbium silicides. The rare earth atom has a minor influence on the calculated frequencies, which is attributed to the atomic mass difference.

[1] B. Halbig et al., Phys. Rev. B 97, 035412 (2018)

[2] S. Sanna et al., Phys. Rev. B 93, 195407 (2016)

O 18.4 Mon 17:45 Poster F

Au atomic wires on Si(hhk) substrates: Recent advances from experiment and theory — •Simone Sanna[1], Zamin Mamiyev[2], Christoph Tegenkamp[3], and Herbert Pfnür[2] — [1]Justus-Liebig-Universität Gießen — [2]Leibniz Universität Hannover — [3]Technische Universität Chemnitz

The investigation of substrate-supported quasi-1D atomic wires flourished in the last decade, owing to recent advances in experimental techniques for surface analysis, and fueled by the growing demand for outstanding materials. While many 1D properties are not spoiled by structural embedding, the coupling to the environment allows modifying physical properties, e.g., the wire metallicity. In this respect, Au wires grown on vicinal Si(111) surfaces are an ideal playground, as the miscut controls the wire width (single or double atomic rows) and the interwire distance. In this contribution, we report on theoretical and experimental studies recently performed to explore the coupling of Au wires on Si(hhk) surfaces with the environment. Adsorption of H and O is found to affect differently single and double Au wires [1]. The coupling of the wires to higher dimensions through the substrate results in the breakdown of the nearly-free electron gas model [2]. Thus, the wires are more appropriately described as extremely anisotropic 2D objects than as purely 1D.

[1] Z. Mamyev et al., Phys. Rev. Mat. 2, 066002 (2018). [2] S. Sanna et al., J. Phys. Chem. C 122, 25580 (2018). [3] Z. Mamyev et al., Phys. Rev. B, submitted.

O 18.5 Mon 17:45 Poster F

Multi-pulse excitation of one-dimensional nanowires at surfaces — •Nils Häusser, Jan Gerrit Horstmann, Hannes Böckmann, and Claus Ropers — IV. Physical Institute, University of Göttingen, Friedrich-Hund-Platz 1, Germany

Steering the making and breaking of bonds in solid-state phase transitions by intense light fields is one of the ultimate goals of ultrafast condensed matter physics. Multi-pulse [1] and resonant [2] optical excitation schemes promise coherent control over structural phase transitions in solids and at surfaces on their inherent time scale. Here, we explore the potential of multi-pulse excitation for inducing and controlling structural phase transitions in low-dimensional materials. Starting with a two-pulse scheme, we investigate and control the structural phase transition in In-nanowires on Si(111) [3]. We find that the transition is governed by the dynamics of only two structural modes, making indium on silicon a model system to study the feasibility of more complex and tailored excitation schemes.

[1] A. M. Weiner et al., Science 247, 1317-1319 (1990). [2] M. Rini et al., Nature 449, 72-74 (2007). [3] T. Frigge et al., Nature 544, 207-211 (2017).

O 18.6 Mon 17:45 Poster F

Simulating organic functionalization of Si(553)-Au — •Conor Hogan[1], Svetlana Suchkova[2], Friedhelm Bechstedt[3], Eugen Speiser[2], Sandhya Chandola[2], and Norbert Esser[2] — [1]Istituto di Struttura della Materia-CNR (ISM-CNR), Rome, Italy — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V. Berlin — [3]Friedrich-Schiller-Universität Jena

Stepped gold-stabilized Si(553) surfaces offer much potential for self-organized assembly of one- and two-dimensional nanostructured arrays of organic molecules [1]. Regular atomic chains of Au and Si on the surface, running parallel to the step edges, act as natural templates for ordered organic functionalization. Strong covalent bonding to the semiconductor substrate determines that layer formation is controlled by the local surface reactivity. In this theoretical study we investigate the adsorption of various simple organic molecules with different functional groups on Si(553)-Au [2]. In particular we investigate the role of the functional group on the final geometry and electronic structure and show that hydrogen co-doping offers a means to tune the local reactivity [3].

[1] S. Suchkova, C. Hogan, F. Bechstedt, E. Speiser, N. Esser, Phys. Rev. B 97, 045417 (2018). [2] C. Hogan, S. Suchkova, F. Bechstedt, E. Speiser, S. Chandola, N. Esser, submitted. [3] C. Hogan, E. Speiser, S. Chandola, S. Suchkova, J. Aulbach, J. Schäfer, S. Meyer, R. Claessen, and N. Esser, Phys. Rev. Lett. 120, 166801 (2018).

O 18.7 Mon 17:45 Poster F

Highly Ordered Metallic Phase of Indium on SiC(0001) — Maximilian Bauernfeind, •Jonas Erhardt, Jörg Schäfer, and Ralph Claessen — Physikalisches Institut and Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany

For the monolayer growth of two-dimensional topological insulators (2D-TIs) on the insulating SiC(0001) substrate, the strong interaction between the deposited layer and the substrate dangling bonds (DBs) plays a pivotal role and drastically affects the electronic structure of the system. Especially 2D-TIs with fragile topology, e.g. quasi-freestanding stanene, require a passivated substrate to cancel out such interactions that are detrimental for the topological properties [1]. Indium with its three valence electrons is such a passivation candidate and leads to metallic or insulating phases on various semiconducting surfaces. Here we report first results of a highly ordered indium phase on SiC(0001). Scanning tunneling microscopy (STM) reveals a Kagome-like superstructure with a lattice constant of approximately 2.1 nm tentatively assigned as a $(4\sqrt{3}\times4\sqrt{3})$R30° reconstruction. Additionally, scanning tunneling and angle-resolved photoelectron spectroscopy (STS and ARPES) show a band structure distinct from pristine SiC and reveal a metallic character with a pronounced electron pocket, indicative of a 2D electron gas. Interestingly, despite the large unit cell observed in STM and low-energy electron diffraction, the corresponding Brillouin zone is not effective in the ARPES band structure.

[1] D. Di Sante et al., arXiv:1807.09006 (2018)

O 18.8 Mon 17:45 Poster F

Sn nanowires on a vicinal Si(111) surface — •Monika Jäger[1], Herbert Pfnür[1], Mauro Franciulli[2], Andrew Weber[2], Jan-Hugo Dil[2], and Christoph Tegenkamp[1,3] — [1]Leibniz Universität Hannover, Germany — [2]Swiss Light Source, Villigen, Switzerland — [3]TU Chemnitz, Germany

The α-Sn phase on Si(111) is a prototype system for a two-dimensional Mott phase. Recently, the low temperature phase was investigated by means of spin-resolved ARPES showing that the formation of the row-wise collinear antiferromagnetically spin-ordering is accompanied by a small Rashba-splitting of the highest occupied Mott state [1].
In order to study the influence of confinement towards the Mott state we studied the growth of Sn-nanowires on vicinal Si(111) by means of STM and ARPES. Depending on the Sn coverage, three different phases were identified. At low coverages, the surface structure of Si(557) is preserved comprising 3 nm wide α-Sn stripes. They exhibit a metallic surface state in ARPES at low temperatures possibly due to doping of the Mott state via step edges. Similar observations of metallic QP states were reported for hole doped α-Sn/Si(111) [2]. Further increase of the coverage to 0.5 ML leads to a refacetting of the surface exhibiting locally a (223) orientation. The wider (111) terraces reveal both $(\sqrt{3}\times\sqrt{3})$ and $(2\sqrt{3}\times2\sqrt{3})$ Sn reconstructions, the latter is well known for 0.3-1.2 ML Sn/Si(111). For higher coverages (>0.7 ML), step bunching sets in resulting in wide $(2\sqrt{3}\times2\sqrt{3})$-domains.
[1] M. Jäger et al., PRB **98**, 165422, (2018).
[2] F. Ming et al., PRL **119**, 266802, (2017).

O 18.9 Mon 17:45 Poster F

Forming and contacting chains of Fe and Co nanoclusters for four-probe transport measurements — •Oleg Kurnosikov[1] and Kongyi Li[2] — [1]Eindhoven University of Technology, Eindhoven, The Netherlands — [2]QuTech, Delft University of Technology, Delft, The Netherlands

Electron transport along a chain of nanoclusters can be governed by a single-electron charge, spin or quantum phenomena as soon the size of the nanoclusters is in the order of several or tens nanometers. To fabricate such system aiming at spin transport we arrange the chains of small Fe and Co nanoclusters on an ultra-thin AlOx layer. Within our approach, the thin oxide layer decouples the electronic states of the nanoclusters from a conductive substrate. Iron and cobalt nanoclusters were obtained by MBE growth at controlled temperature in UHV. The arrangement of the clusters in chains is achieved by exploiting a preferable nucleation along the structural defects of AlOx or, alternatively, by relocation of the individual nanoclusters with the STM tip. However, a direct contacting the chains of nanoclusters for current transport measurements with the four-probes method is not trivial since the contacting process becomes destructive on this scale both for the clusters and thin alumina layer. To solve the problem of 4-probe contacting to the chain we introduced auxiliary gold islands of bigger size mediating the contacts with four probes. Various ways of formation of the gold islands providing the reliable contacts have been tried.

O 18.10 Mon 17:45 Poster F

Surface dependent analysis of freestanding GaAs-nanowires — •Andreas Nägelein[1], Juliane Koch[1], Matthias Steidl[1], Stefan Korte[2], Bert Voigtländer[2], Peter Kleinschmidt[1], and Thomas Hannappel[1] — [1]Institute of Physics, TU Ilmenau, 98693 Ilmenau, Germany — [2]Peter Grünberg Institut (PGI-3,) Forschungszentrum Jülich, 52425 Jülich, Germany

Nanostructures e.g. III-V nanowires (NW) are known as promising candidates for optoelectronic applications. In this work we investigate single, freestanding "vapor liquid solid" (VLS) grown GaAs-NWs by a multi-tip scanning tunneling microscope (MT-STM). Here, four-point probe measurements are performed non-destructively by contacting three tips at the nanowire and using the substrate as a fourth contact. Besides the investigation of doping profiles, a comparison between nanowires prior to and after oxidation was carried out. The resistance slope in the intrinsic part of the NW increased drastically with oxidation. In contrast to doped NW-parts where the charge carrier transport mainly takes place in the center of a NW, a conductive channel does not exist for intrinsic NWs. Besides contamination-induced band bending, the conductivity is also affected by the surface states themselves. Since oxidation changes the surface states and thereby the space charge layer, we consider a changed surface conductivity of the intrinsic nanowire segment as a likely explanation of its increased resistance after exposure to ambient atmosphere.

O 18.11 Mon 17:45 Poster F

Tailor-made *meso to macro* porous CuNi films by electrodeposition: synthesis and application — •Jin Zhang[1,2], Jordi Sort[2,3], and Eva Pellicer[2] — [1]State Key laboratory of Solidification Processing, Center of Advanced Lubrication and Seal Materials, Northwestern Polytechnical University, Xi'an, Shaanxi, 710072, P. R. China — [2]Departament de Física, Universitat Autònoma de Barcelona, E-08193 Bellaterra, Spain — [3]ICREA, Pg. Lluís Companys 23, E-08010 Barcelona, Spain

Porous films with interconnected pores of different dimensions are attractive in many fields like catalysis, gas adsorption, or energy storage, etc. Template-assisted electrodeposition (ED) is very effective to fabricate porous films since meso- to macro-scale pores can be obtained by changing templates. In this talk, the production of macroporous CuNi films by hydrogen bubble-assisted ED is demonstrated. The synthetic approach results in porous films with highly interconnected nanodendritic walls[1]. Moreover, P123 tri-block copolymer is used for the ED of mesoporous CuNi films. Pores between 5 nm and 20 nm and dissimilar space arrangements are obtained depending on the parameters[2]. These meso- to macro-porous CuNi films exhibit enhanced electrocatalytic activity towards hydrogen evolution reaction. From a technological point of view, they can also be used as scaffold to host other functional materials that could bring hydrophilic/hydrophobic properties, electrical insulation or even enhanced mechanical performance.

[1] Nanoscale 2014, 6, 12490. [2] ACS Appl. Mater. Interfaces 2018, 10, 14877

O 19: Poster Monday: Organic Molecules on Inorganic Surfaces

Time: Monday 17:45–20:00 Location: Poster F

O 19.1 Mon 17:45 Poster F

On the adsorption behavior of free base tetranaphthylporphyrin on Cu(111): mobility, intramolecular conformation and chirality — •Stephen Massicot, Jan Kuliga, Rajan Adhikari, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The controlled fabrication of molecular nanoarchitectures via bottom-up approach is an important objective within surface science. One of the most promising and extensively investigated class of adsorbates in that regard are porphyrins. In order to understand the adsorption behavior of porphyrins one has to closely study their adsorption geometry. In this study, we investigate the free-base tetranaphthylporphyrin (2HTNP) on Cu(111). Interestingly, 2HTNPs adsorb as individual molecules exhibiting an "inverted" conformation on the copper substrate, similar to the reports for the tetraphenylporphyrin. However, each napthyl group of a single 2HTNP molecule has two different orientations parallel to the surface. As a result five atropisomeric and two enantiomeric conformations can be found. Furthermore, a specific dynamic behavior, i.e. a migration of the adsorbed 2HTNP molecules along the three high symmetry regions of the substrate is observed at room temperature. After annealing to 400 K only one conformation is present on the surface and the molecules are static. However, after further annealing to 450 K the molecules become mobile again and some molecules additionally change the substrate directions.

O 19.2 Mon 17:45 Poster F

Adsorption Geometry of 2-Iodotriphenylene on Ag(111) — •Alexander Ihle[1], Daniel Martin-Jimenez[1], Daniel Ebeling[1], Hermann Wegner[2], Tobias Schlöder[3], Doreen Mollenhauer[3], and André Schirmeisen[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Germany — [2]Institute of Organic Chemistry, Justus Liebig University Giessen, Germany — [3]Institute of Physics and Chemistry, Justus Liebig University Giessen, Germany

On-surface chemistry is a powerful tool for building covalent molecular structures such as chains, networks, or graphene nanoribbons [1, 2]. In particular, the catalytic properties of the metal substrate as well as the 2D confinement facilitate the synthesis of new structures that are not accessible via solution chemistry. In order to control the bottom-up formation process precise knowledge about the adsorption geometry of the molecular precursors is needed since this will help to understand the reaction mechanisms in detail. Here we studied the adsorption geometry of 2-iodotriphenylene on Ag(111). By using low temperature atomic force microscopy with CO-functionalized tips we are able to identify the adsorption position and angles with high precision. Only two orientations are observed on the surface which is attributed to relatively strong molecule-substrate interactions.

[1] Cai, J. *et al.* *Nature* **466**, 470-473 (2010)

[2] Grill, L. *et al.* *Nature Nanotechnology* **2**, 687-691 (2007)

O 19.3 Mon 17:45 Poster F

Scanning Tunneling Microscopy Study of Phthalocyanine Family Molecule with Reactive Moiety of Thiadiazol: Cobalt tetrakis (1,2,5-thiadiazole) porphyrazines(CoTTDPz) adsorption on Au(111) — •Yu Wang[1,3], Jie Hou[1,3], Kunio Awaga[2], and Tadahiro Komeda[3] — [1]Department of Chemistry, Graduate School of Science, Tohoku University, Aramaki-Aza-Aoba, Aoba-Ku, Sendai, Japan — [2]Department of Chemistry & Research Center for Materials Science, Nagoya University, Chikusa-ku, Nagoya, Japan — [3]Institute of Multidisciplinary Research for Advanced Materials (IMRAM, Tagen), Tohoku University, 2-1-1, Katahira, Aoba-Ku, Sendai, Japan

Metal-phthalocyanine(MPc) has been intensively studied in recent decades not only for its chemical and thermal stability but also due to tunable properties through using various center metal atoms. Here we report a LT-STM study of Pc family molecule: CoTTDPz, the terminal of ligand is S-N instead of carbon in Pc, indicating a strong lateral interaction between molecules. CoTTDPz is deposited on Au(111) substrate using thermal sublimation method, multiple molecule layers from 1st to 3rd can be distinguished from STM images. First layer molecules have two orientations which is different with previous works for MPc, noted that first layer molecules had a unique orientation. In second layer, CoTTDPz shows two types of tilted configurations which can be judged from image and STS. Third layer molecules have two similar configurations absorbed on type1 and type2 of second layer, which has never been reported on Pc molecules.

O 19.4 Mon 17:45 Poster F

Investigation of Self-Assembend Caffeine Monolayer Formation on Au(111) — •Malte Schulte[1,2], Ismail Baltaci[1,2], Peter Roese[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4a, 44227 Dortmund, Germany — [2]DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund, Germany

In recent years the molecule caffeine gained particular interest due to its importance in pharmaceutical applications. The bioavailability of particular substances can be tuned by their structure. Furthermore, in bulk crystals caffeine shows a polymorph behavior with a stable β- and a metastable high-temperature α-phase. Moreover, an analysis of substrate induced caffeine crystalline growth on different substrates was done recently. Therefore an investigation of caffeine monolayer growth can reveal insides of the crystallite growth and gives details about different phases.

In order to study these aspects from a bottom-up approach we deposited caffeine molecules on an Au(111) surface under ultra-high vacuum conditions. To investigate the monolayer self-assembly of caffeine molecules on this surface we performed Scanning Tunneling Microscopy (STM), Low Energy Electron Diffraction (LEED) and X-ray Photoelectron Spectroscopy (XPS). Our results demonstrate successful caffeine monolayer formation, including an molecular alignment in two different directions the Au(111) surface.

O 19.5 Mon 17:45 Poster F

Heteromolecular interfaces on metals in the physisorptive regime — •Qi Wang[1], Antoni Franco-Canellas[1], Jiacheng Yang[2], Samuel Struzek[1], Mengting Chen[2], Steffen Duhm[2], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [2]Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, China

Bilayers of pi-conjugated organic molecules, being considered as model systems for more complex thin film architectures, have been used to investigate the templating effect on metals. Because molecular exchange can hamper the controlled preparation of heteromolecular structures [1], a detailed characterization of different molecule-substrate combinations is required. We found that the organic-metal interaction strength is the decisive factor for the favorable sequential arrangement in organic heterostructures and molecular exchange is possible to occur for weakly interacting template layers [1]. To investigate the molecular arrangement in a physisorptive regime, we have studied the vertical arrangement and the chemical fingerprints of two bilayer systems deposited on Au(111) surfaces [2]. The adsorption properties of organic systems were investigated by X-ray standing waves (XSW), X-ray photoelectron spectroscopy (XPS), ultraviolet photoelectron spectroscopy (UPS).

[1] Q. Wang, et.al. J. Phys. Chem, C. 2018, 122, 9480-9490.
[2] A. Franco-Canellas, et.al. Phys. Rev. Mater. 2017, 1, 013001.

O 19.6 Mon 17:45 Poster F

Diels-Alder adduct formation of pentacene and C_{60} on graphene/Ru(0001) and Cu/Ru(0001) — •Sebastian Flade and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

The combination of pentacene and C_{60} represents a prototypical donor-acceptor system that is ideal to study fundamental processes in organic photovoltaics. Very recently, an efficient Diels-Alder adduct formation at the heterolayer interface has been reported.[1] Using infrared-absorption spectroscopy we have unambiguously identified the reaction product and investigated the kinetics of this reaction. Specifically, the thermal evolution of the formation and decomposition of the C_{60}-PEN adduct has been examined. Another aspect concerned the dependence on layer thickness and stacking sequence which seem to play an only minor role for the described (reversible) interface reaction. We demonstrate that the reaction likewise proceeds when one of the reaction partners is in direct contact with the substrate. This has been verified for inert substrates like graphene/Ru(0001), as well as the more reactive Cu/Ru(0001) template.

[1] T. Breuer et al., Adv. Mater. Interfaces 3 (2016) 1500452.

O 19.7 Mon 17:45 Poster F

X-Ray Small Angle In-Situ Study of Porphyrin Adsorption on Stabilized Rutil SurfacesX-Ray Small Angle In-Situ Study of Porphyrin Adsorption on Stabilized Rutil Surfaces — •Klaus Götz, Annemarie Pfnür, and Tobias Unruh — Institute for Crystallography and Structural Physics, Erlangen, Germany

Dye sensitized solar cells (DSSCs) based on TiO2 have been studied as an easy to produce, low-cost alternative to classical semiconductor solar cells with recent efficiencies of up to 13% for a long time [1][2]. We synthesized tunable titania nanoparticles with a diameter of 2-3 nm that are stabilized by oleic acid. Special emphasis of our work is focused on the exchange process of the oleic acid with porphyrins designed for a particular application.

This process is studied using a variation of different x-ray small angle scattering techniques. One method is the combination of small angle x-ray and neutron scattering (SAXS and SANS) experiments. These are well suited to study core/shell systems because of the different scattering lengths for x-rays and neutrons. On the other hand x-ray reflectivity measurements can be used to study layered systems on flat substrates. This offers the possibility to study the exchange of oleic acid with porphyrins on TiO2 Wafers as a test system. The poster will give an overview over the different techniques and their usage in the characterization of the morphology of the produced particles and the ligand exchange from oleic acid to porphyrins.

[1] O'Regan & Grätzel; Nature 353, 737-740 (1991)
[2] Matthew S. et al.; Nat. Chem. 6; 242-247 (2014)

O 19.8 Mon 17:45 Poster F

Quantitative Determination of a Model Organic/Insulator/Metal Interface Structure — Martin Schwarz[1], David A. Duncan[2], Manuela Garnica[1], Jacob Ducke[1], Aleksandr Baklanov[1], Peter S. Deimel[1], Johannes Küchle[1], Pardeep K. Thakur[2], Tien-LIn Lee[2], Francesco Allegretti[1], and •Willi Auwärter[1] — [1]Technical University of Munich, Germany — [2]Diamond Light Source, U.K.

Two-dimensional epitaxial materials including hexagonal boron nitride (hBN) are frequently employed as templates for self-assembled molecular films and nanostructures [1]. A quantitative structural characterization of the respective interfaces and adsorbate geometries however is largely missing. Here, we report on the geometric and electronic structure of a prototypical organic/insulator/metal interface, namely metallo-porphines (Co-P, Zn-P) on monolayer hBN on Cu(111), investigated by combining X-ray photoelectron spectroscopy, X-ray standing waves and scanning tunneling microscopy [2]. Specifically, we determine the adsorption height of the organic molecules and show that the original planar molecular conformation is preserved in contrast to the adsorption of Co-P on Cu(111) [3]. In addition, we highlight the electronic decoupling provided by the hBN spacer layer and find that the hBN-metal separation is not significantly modified by the molecular adsorption.

[1] W. Auwärter, Surf. Sci. Rep., doi:10.1016/j.surfrep.2018.10.001
[2] M. Schwarz, et al., Nanoscale 10, 21971 (2018)
[3] M. Schwarz, et al., J. Phys. Chem. C 122, 5452 (2018)

O 19.9 Mon 17:45 Poster F

On-Surface Synthesis and Characterization of Lanthanide and Actinide Tetrapyrrole Complexes — •Erik Rheinfrank, Mathias Pörtner, Carmen N. Beyerle, Peter Feulner, Peter S. Deimel, Felix Haas, Francesco Allegretti, Johannes V. Barth, and Willi Auwärter — Technical University of Munich, Germany

Metal-organic complexes and coordination architectures on metal surfaces have attracted considerable interest. Specifically, lanthanide-based structures provide distinct structural, electronic, and magnetic properties [1], whereas actinides are rarely explored to date. Lanthanides and actinides can be sandwiched between macrocyclic ligands, resulting in 3D complexes, such as tetrapyrrole double- and multideckers [1]. Here, we report on the in-situ synthesis of Th-TPP complexes on a Ag(111) surface under ultra-high vacuum conditions by exposing a tetraphenylporphyrin (TPP) multilayer to an atomic beam of Th followed by a temperature-programmed reaction and desorption of surplus material. The nature of the interaction between Th and the TPP molecules, as well as the electronic properties of this metal-organic compound were investigated using X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS). The findings will be discussed in relation to Ce-based complexes, such as Ce-phthalocyanine sandwich compounds.

[1] D. Ecija et al., Acc. Chem. Res. 51, 365 (2018)

O 19.10 Mon 17:45 Poster F

Adsorption of organic molecules with high dipole moment on the Au(111) surface — •Tobias Müller[1], Philipp Rietsch[2], Siegfried Eigler[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Institute for Chemistry and Biochemistry, FU Berlin

Molecules with high dipole moment exhibit promising electronic properties for possible single-molecule electronic devices [1]. Of particular interest is how they couple to conducting substrates and how this coupling changes electronic states and intramolecular charge distribution.

To obtain first insights into the behavior of such high dipole molecules on a metallic substrate we have studied the adsorption of N2-Ethan-Tetracyanoquinodimethan and N2-Benz-Tetracyanoquinodimethan on a Au(111) surface using density functional theory (DFT). We have identified the preferred adsorption sites and molecular orientations on the surface and we determined possible periodic arrangements for dipolar stripes. Calculated scanning tunneling microscopy (STM) and local contact potential difference (LCPD) images will be presented and changes in the electronic structure of the molecules within the dipolar stripes will be discussed.

[1] P. Rietsch, F. Witte, S. Sobottka, B. Sarkar, B. Paulus, U. Resch-Genger, S. Eigler, *Diaminodicyanoquinone: A Novel Class of Fluorescent Electron Acceptor Dyes with High Dipole Moments*, submitted

O 20: Poster Monday: Electronic Structure

Time: Monday 17:45–20:00 Location: Poster F

O 20.1 Mon 17:45 Poster F

CuI as Potential *p*-type Transparent Conductor: Electronic and Optical Properties from First Principles — •Michael Seifert, Claudia Rödl, and Silvana Botti — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The lack of viable *p*-type transparent conductors represents a critical bottleneck for future transparent electronics. CuI, with its direct band gap of 3.1 eV and its demonstrated *p*-type conductivity, is a promising candidate for such a material. Recently, it has raised significant renewed interest due to the production of transparent conducting bipolar CuI/ZnO heterostructure diodes, its applications as hole collection layer in organic electronics, or as promising candidate for a flexible, transparent thermoelectric material. However, a detailed theoretical understanding of the optical properties of CuI is still missing.

We use density-functional theory and many-body perturbation theory to study the structural, elastic, electronic, and optical properties of CuI in the zincblende structure (also known as the room-temperature γ phase). We have calculated key quantities of its electronic structure, in particular the band gap, effective electron and hole masses, and spin-orbit-coupling induced band splittings and compare them to available experimental values. Furthermore, we explore the optical absorption properties in the vicinity of the band gap heading towards the inclusion of excitonic effects.

O 20.2 Mon 17:45 Poster F

Hybrid functionals with self-consistent density-dependent mixing — •Thorsten U. Aull, Ahmad W. Huran, and Miguel A. L. Marques — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale) Germany

One of the most famous deficiencies of Kohn-Sham density functional theory is the systematic underestimation of band gaps when they are approximated as the difference between the Kohn-Sham eigenvalues of the highest occupied eigenstate and the lowest unoccupied one [1]. Calculations with conventional hybrid functionals result in reasonable band gaps for many materials, however, within a rather narrow window for the gap [2]. This problem is attributed and large to the fact that the mixing parameter is a constant. In the work of Marques *et al.* it was shown that a suitable system-dependent mixing parameter can be estimated as a functional of the density of the system at hand [2]. Thus, the amount of the Hartree-Fock exchange energy is by far not the same for every material. Since the derivation of their mixing parameter was done at the level of the exchange-correlation potential, we study the limits of the proposed mixing parameter and show the requirements for self-consistent calculations using such an approach to gain access to energetic properties.

[1] J. Perdew, Int. J. Quantum Chem. **28**, 497 (1985).
[2] M. Marques *et al.*, Phys. Rev. B **83**, 035119 (2011).

O 20.3 Mon 17:45 Poster F

Analysis of defect states in MoSe$_2$ and unfolding of defect band structure — •Stefan Rost, Christoph Friedrich, Irene Aguilera, Beata Kardynal, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We identify possible dopants in MoSe$_2$ that could facilitate single photon emission reflecting the symmetry of the host lattice. In particular, we investigate dopants in the chalcogen layer, because these are easiest to implant and introduce only little strain on the crystal structure. Suitable dopands are identified by density-functional-theory (DFT) studies of structural relaxation, projected density-of-states, band structure, and electron energy loss spectra, all calculated with the Jülich FLAPW code family. Calculations for the doped systems are performed using a super-cell that contains 3×3 monolayer MoSe$_2$ unit cells. Due to the breaking of translational symmetry, it is difficult to interpret the band structure of defect systems, in particular, for low doping concentrations. Therefore, we implemented a method for unfolding the bands in the Fleur code (www.flapw.de). The resulting band structure resembles the one of the pristine material, but it contains additional information about the defect states and their interaction with the MoSe$_2$ bands. It is shown that doping with group-5 and group-7 elements is promising. To understand the many-body effects on the defect level, *GW* corrections are calculated.

We acknowledge the support through "Integration of Molecular Components in Functional Macroscopic System" initiative of VW Stiftung.

O 20.4 Mon 17:45 Poster F

Electronic and Optical Properties of Pb and Sn Based Halide Perovskites from First Principles — •Cecilia Vona[1], Dmitrii Nabok[1], and Claudia Draxl[1,2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]European Theoretical Spectroscopic Facility (ETSF)

Organic - inorganic metal halide perovskites have emerged as promising materials for next generation solar cells. However, the compounds with optimal light-harvesting properties contain lead. Therefore, a non-toxic metal that can replace Pb, without drastically decreasing the devices performance, needs to be found. Sn-based perovskites are studied as possible candidates, but their properties are not comparable with the Pb-based counterpart. To understand the different behavior of these materials, we analyze and compare their electronic and optical properties by performing first-principles calculations with the all-electron full potential code `exciting`. The electronic properties are computed in the density-functional-theory framework. The impact of different exchange-correlation functionals is investigated, and particular attention is paid to the effect of spin-orbit coupling. To get insight into the origin of the observed optical excitations, including excitonic effects, we compute the absorption spectra of Pb- and Sn-based perovskites by solving the Bethe-Salpeter equation.

O 20.5 Mon 17:45 Poster F

Towards efficient GW calculations in magnetic systems — •Masoud Mansouri[1,2], Peter Koval[1,2], and Daniel Sanchez-Portal[1,2] — [1]Donostia International Physics Center (DIPC) — [2]Centro de Física de Materiales, Centro Mixto CSIC-UPV/EHU, Paseo Manuel de Lardizabal 5, 20018 Donostia-San Sebastián, Spain

Hedin's *GW* approximation *GW*A has gained popularity in the material science community because of its high quality and relatively low computational cost. A prerequisite to describe magnetic materials is the capability to describe systems containing unpaired electrons. However, spin-resolved *GW* calculations for electronic systems with unpaired electrons have not yet been extensively developed.

In this work, we benchmark unrestricted *GW*A for open-shell molecules. We perform one-shot G_0W_0 calculations for 42 small molecules belonging to the G2/97 test set. As reference we use the Gold standard of quantum chemistry, namely coupled cluster singles, doubles, and perturbative triples. Both reference CCSD(T) and *GW* calculations are performed using Dunning's correlation-consistent basis sets expanded in terms of Gaussian functions. This benchmarking indicates deviations smaller than 0.5 eV, which is comparable to those found for closed-shell molecules. Furthermore, we do not find a clear connection between the spin contamination and this deviation. The results are encouraging for the use of Hedin's *GW*A for magnetic materials in combination with basis sets of atomic orbitals.

O 20.6 Mon 17:45 Poster F

CO Oxidation by noble metal single atom catalysts on transition metal doped oxides — •Debolina Misra and Satyesh Yadav — Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India

Stability of transition metal (TM) defects in BaO and MgO have been studied using density functional theory. Our defect formation energy calculations show that TM atoms at various charge states can be stabilized not only at the substitutional sites, but some of them can also be accommodated well in the tetrahedral voids available in the oxides. We use this result to solve the problem of binding noble metal atoms in heterogeneous catalysis by proposing a new and effective way to anchor them on the support material. Single atoms of Pt, Pd and Au are considered on TM (Nb, Mo) doped BaO {001} surface for CO oxidation. Both hollow (H) and O-top (O) positions of the oxide surface are considered as the possible binding sites for the metal atoms. Our results reveal that compared to bare BaO {001} surface, noble metals bind more strongly when the surface is doped by Nb or Mo. For example, binding energy of Au changes from -1.28 eV (H) and -1.85 eV (O) in BaO {001}, to (i) -3.61 eV (H) and -3.69 eV (O) in Nb-doped, and (ii) -3.57 eV (H) and -3.70 eV (O) in Mo-doped {001} surface. This is attributed to the charge transfer between TM dopants and the noble metal atoms. Our calculated adsorption energies of CO molecule on the noble metal atoms are comparable to other catalytically active systems. We further calculate the minimum energy pathway and the reaction barriers for all the elementary steps of CO oxidation.

O 20.7 Mon 17:45 Poster F

Electronic structure of epitaxially grown topological insulator (Bi,Sb)$_2$Te$_3$ films with varying magnetic doping. — •Sonja Schatz[1], Ali Al-Janabi[1], Maximilian Rudloff[1], Celso Fornari[1], Thiago R. F. Peixoto[1], Hendrik Bentmann[1], Steffen Schreyeck[2], Martin Winnerlein[2], Charles Gould[2], Karl Brunner[2], Laurens W. Molenkamp[2], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Experimentelle Physik III, Universität Würzburg, D-97074 Würzburg

Topological insulators (TI) have gained great interest over the last years. In particular, the topological properties of the ternary compound (Bi,Sb)$_2$Te$_3$ can be varied via doping with magnetic impurities. The magnetic doping of TI thin films is especially interesting, due to the formation of a ferromagnetic ground state, which leads to the arising of the quantum anomalous Hall state at low temperatures.

In this work we explore the electronic structure of (Bi,Sb)$_2$Te$_3$ films grown on BaF$_2$ (111) by angle-resolved photoelectron spectroscopy (ARPES) experiments. The nearly perfect lattice match between film and substrate results in homogenous films and ARPES data of high quality. Besides results on pristine thin films we will also present measurements on (Bi,Sb)$_2$Te$_3$ layers doped with magnetic impurities, for which an exchange splitting of the topological surface state is expected in the ferromagnetic state.

O 20.8 Mon 17:45 Poster F

Observation of surface and bulk charge density waves in LaTe$_3$ — Shuvam Sarkar[1], Pampa Sadhukhan[1], •Davide Curcio[2], Marco Bianchi[2], Arnab Pariari[3], Shubhankar Roy[3], Prabhat Mandal[3], Philip Hofmann[2], and Sudipta Roy Barman[1] — [1]UGC-DAE Consortium for Advanced Scientific Research, Indore, India — [2]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [3]Saha Institute of Nuclear Physics, Kolkata, India

LaTe$_3$ is a model Charge Density Wave (CDW) material of the rare-earth tritelluride family, with an anisotropic CDW that has a transition temperature higher than 450 K [1]. The layered structure is furthermore anisotropic, resulting in a CDW that is preferentially one dimensional: A large bandgap of 0.4 eV exists along one direction, but at the same time metallic states are present in the perpendicular direction even below the CDW transition temperature [2].

The spectral function of this material has been measured by angle resolved photoelectron spectroscopy (ARPES), including the $k_\perp$ dispersion, giving access to the full 3-dimensional band structure.

In this experimental ARPES study, we show how the CDW can be largely accounted for by nesting of wave vectors at the Fermi surface.

[1] N. Ru *et al.*, Phys. Rev. B **77**, 035114 (2008)

[2] V. Brouet *et al.*, Phys. Rev. B **77**, 235104 (2008)

O 20.9 Mon 17:45 Poster F

Optimization of a numerical integration procedure for the Korringa-Kohn-Rostoker Green's function method — •Irina Heinz, Alexander Fabian, Philipp Risius, and Christian Heiliger — Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Gießen

For the description of material properties an efficient calculation of the density of states and charge density is invaluable. We calculate these quantities based on density functional theory (DFT) within the framework of the Korringa-Kohn-Rostoker (KKR) Green's function method. This method requires integrating the Green's function within a certain energy interval. However, due to the strongly structured Green's function the numerical integration requires a lot of computational effort. Therefore, integration is typically performed in the complex energy plane.

In the present case, we consider a rectangular contour in the complex energy plane. The numerical effort required depends on the position along the contour, particularly the imaginary part of the complex energy. In order to obtain reasonable numerical accuracy in conjunction with affordable computational time, we thoroughly analyze the dependence of the integral on certain numerical parameters such as the density of the k-mesh in reciprocal space and the choice of the energy grid along the integration contour.

O 20.10 Mon 17:45 Poster F

Calculation of non-equilibrium occupation function — •Jonas Fey, Jonas F. Schäfer, Alexander Fabian, Philipp Risius, Michael Czerner, and Christian Heiliger — Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

The development of new nanoscale devices requires a precise theoretical description. This can be realized within the Keldysh formalism by means of non-equilibrium Green's functions. In order to increase the accuracy or number of these calcuations the numerical effort should be kept as low as possible. In the case that the occupation function of the system is known the numerical effort can be decreased by allowing the energy to take complex values and using the residue theorem to calculate an occuring integral along paths in the complex energy plane. This is for example the case for equilibrium systems. We were able to show that for a simple model system this trick can be extended to non-equilibrium. By applying the Keldysh formalism to complex valued energies one obtains an equation to calculate the occupation function. The effects of this method on the numerical effort were examined depending on the desired accuracy.

O 20.11 Mon 17:45 Poster F

Revealing the role of the interface in the high-temperature superconductivity of single-layer FeSe/SrTiO$_3$ — •Rui Peng — Advanced Materials Lab, Fudan University, Shanghai, China

Interface hosts unexpected physics due to competing orders, charge transfer, strain and other degrees of freedom for quantum interactions. At the interface between monolayer FeSe films and SrTiO$_3$, the superconducting transition temperature (Tc) is unexpectedly high. The mechanism for the Tc enhancement has been the central question, as it may present a new strategy for seeking out higher Tc materials. In this talk, I will introduce the series of our work on the FeSe/oxide interface involving electronic structure studies using in-situ ARPES, atomic-scale structural studies using STEM and synchrotron SXRD, and interface atomic-scale engineering using oxide MBE and MBE. We systematically reveal the relationship between superconductivity and various interfacial interactions, including strain, thickness, carrier doping, interfacial phonon energy, and interfacial electron-phonon coupling strength. Striking evidence is observed that the high Tc in FeSe/SrTiO$_3$ is the cooperative effect of the intrinsic pairing mechanism in the FeSe and interactions between the FeSe electrons and SrTiO$_3$ phonons. Moreover, we enhanced the superconducting pairing temperature of single-layer FeSe to 75K, which is a new record of pairing temperature for Fe-based superconductors and monolayer-thick films. Our results point to the promising prospect that similar cooperation of Cooper pairing channels may be a general framework to understand and design high-temperature superconductors.

O 21: Poster Monday: Plasmonics and Nanooptics

Time: Monday 17:45–20:00 Location: Poster F

O 21.1 Mon 17:45 Poster F

Comparing resonance tuning of infrared rod and slit antennas enabled by phase-change materials — •Lukas Voelkel, Achim Strauch, Andreas F. Hessler, Matthias Wuttig, and Thomas Taubner — Institute of Physics (IA) RWTH Aachen

Phase-change materials (PCMs) have been shown to be a useful tool to provide metasurfaces with an active functionality. Since they generally have large optical contrasts between their metastable amorphous and crystalline phases, a change in the phase of a thin film of PCM greatly influences the optical response of a metasurface [1]. This phase-change can be controlled very locally around individual nanostructures with a focussed pulsed laser by either using long, low-energy or short, high-energy pulses for crystallization or amorphization, respectively [2].

In our work, we investigate the switching of nanostructures with PCM $Ge_3Sb_2Te_6$. Because rod and slit antennas response to excitation with completely different near-field distributions, we compare their switching behavior and further demonstrate continuous tuning of the resonance frequency of the nanostructures.

A complete understanding of the switching process of the PCM is the basis for an efficient design of versatile metasurfaces suitable for nanophotonic applications.

[1] M. Wuttig et al., Nat. Photon. 11, 465 (2017)
[2] P. Li et al., Nat. Mater. 15, 870 (2016)

O 21.2 Mon 17:45 Poster F

Coupling of Quantum Dots to Plasmonic Slot Waveguides — •Lok-Yee Yan, Mike Prämassing, and Stefan Linden — Physikalisches Institut, University of Bonn, Nußallee 12, D-53115 Bonn, Germany

Quantum emitters coupled to plasmonic systems are considered as promising candidates for building blocks in quantum plasmonic circuits. So far, several plasmonic platforms such as silver nanowires and gold V-grooves have been exploited. These concepts rely on the tight electric field confinement, hence an enhanced coupling of quantum emitters to the mode, and the guided radiation in the form of plasmon modes. We report on the fabrication of a hybrid system consisting of colloidal CdSeTe-quantum dots (QDs) and a 100 nm wide slot waveguide milled into a thermally evaporated 50 nm thick gold film. We use standard electron beam lithography in combination with an alignment process to deposit the QDs into the slot. The colloidal QDs are provided with carboxyl surface groups which enable chemical bonding to the sample surface. The QDs can launch guided surface plasmons in the slot which induce scattered photons at the end of the slot. Moreover, QDs deposited in the slot region experience an increase of the local photonic density of states which leads to a lifetime reduction of excited states. We demonstrate the coupling of QDs to the slot mode by imaging the fluorescence of the QDs onto an EMCCD camera and showing a reduction of lifetime.

O 21.3 Mon 17:45 Poster F

Optical ratchet based on plasmonic waveguide arrays — •Zlata Cherpakova and Stefan Linden — Physikalisches Institut, Universität Bonn, Nußallee 12, 53115 Bonn, Germany

A ratchet is a spatially periodic system in which the directional transport of particles is achieved without a bias force. Based on the quantum-optical analogy, we propose a new design of a plasmonic ratchet and demonstrate directional transport of surface plasmon polaritons (SPPs). Our design resembles the time-dependent version of the Rice-Miele model: the couplings (i.e. the distances) between the adjacent waveguides and effective refractive indices (i.e. heights) are changing periodically. The plasmonic structures are fabricated by making use of negative-tone gray-scale electron beam lithography. SPPs are excited by shining a highly focused laser beam on the grating, deposited on top of the central waveguide. The spatial evolution of surface plasmon polaritons (SPPs) in the arrays is monitored by the leakage radiation microscopy. One observes an efficient directional transport of SPPs in such an array in a single preferred direction. Additional refractive index variation distinguishes our system from a simple combination of directional couplers. We show that even a very small height variation makes the SPP transport independent on the period of modulation. The role of the phase offset $\Delta\phi$ between the refractive index modulation and coupling modulation is investigated, the maximum transport efficiency is reached for $\Delta\phi = \pi/2$

O 21.4 Mon 17:45 Poster F

Switchable cavity-assisted energy transfer in the infrared via surface phonon polaritons — •Mohsen Janipour[1], Matthias Hensen[2], and Walter Pfeiffer[1] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, Bielefeld 33615, Germany — [2]Physikalische Chemie, Universität Würzburg, Am Hubland, Würzburg, Germany

Devices providing switchable energy and/or signal transfer in the infrared frequency range are essential to realize novel integrated photonic circuits. In the infrared and terahertz regime, Silicon-Carbide (SiC) supports the low-loss surface phonon polaritons. Based on finite difference time domain simulations we investigate high-quality tunable photonic modes in an elliptical metal-SiC heterostructure cavity which serves as a low-loss transfer channel for efficient coupling between two spatially separated locations in the cavity. Tuning of such modes in the Reststrahlen band of SiC is achieved via the longitudinal optical phonon resonance that depends on the carrier concentration. We demonstrate photonic mode shifts larger than 20 times the mode line width and conclude that these cavity modes are well suited to realize optically switchable resonant energy transfer channels in the range between 24-29 THz.

O 21.5 Mon 17:45 Poster F

Investigations of angle-dependent reflection spectra of large-area, disordered perfect absorber structures with ultra-broad absorption — •Ramon Walter[1], Matthias Zilk[2], Izzatjon Allayarov[1], Rostyslav Semenyshyn[1], Gabriel Schnoering[3], Audrey Berrier[3], Thomas Pertsch[2], Thomas Weiss[1], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart — [2]Institute of Applied Physics, Friedrich-Schiller University Jena — [3]1st Physics Institute, University of Stuttgart

So-called perfect absorber devices have the potential for many applications, such as light trapping, photocatalysis, and gas sensing. Such systems show very high absorption at their plasmonic resonance wavelength by optimizing their system impedance to vacuum values. Such perfect absorbers can keep their high absorption over a wide range of the incident angle when gratings mode are suppressed by a disordered arrangement of the plasmonic nanostructures, nearly independent of the polarization of the incoming light.

In this work, we investigate the potential of such devices with a very high absorption over a wide wavelength range, fabricated by colloidal Lithography. To approaches are possible, using a metal with a very broad plasmonic resonance, or creating perfect absorber system with multiple resonances, by using nanospheres of different sizes. We compare these two approaches and investigate the optical properties of the resulting devices under a wide range of incident angles.

We believe that our investigation can lead to improved designs with the potential for many applications.

O 21.6 Mon 17:45 Poster F

Optical tweezers with high-efficiency dielectric metalenses — •Christian Schlickriede[1], Teanchai Chantakit[1], Basudeb Sain[1], Heinz-Siegfried Kitzerow[1], Thomas Zentgraf[1], and Nattaporn Chattham[2] — [1]Universität Paderborn, Paderborn, Germany — [2]Kasetsart University, Bangkok, Thailand

In this work, we present a highly efficient all-dielectric metalens, which is able to optically trap polystyrene microbeads by tightly focusing the incident near-infrared light. In order to achieve a suitable numerical aperture, we use the concept of a geometric phase emerging from the configuration of rotated silicon meta-atoms. This intuitive and flexible design allows various application possibilities, for example multidimensional particle control by complex light fields. Depending on the incident circular polarization of light, the phase profile can be switched between convex and concave which makes this lens also a suitable candidate for polarization dependent particle trapping and antitrapping. In the experiments, we determine the trapping force exerted on the particles and we demonstrate three dimensional particle manipulation. With these results, we demonstrate metasurface enhanced optical tweezers with a broad range of applications in a very compact lab-on-a-chip-ready design.

O 21.7 Mon 17:45 Poster F

Multichannel holographic display and encryption using all-dielectric metasurfaces — •Basudeb Sain[1], Lingling Huang[2], and Thomas Zentgraf[1] — [1]Department of Physics, University of Paderborn, Warburger Straße 100, 33098 Paderborn, Germany — [2]Laser Micro/Nano-Fabrication Laboratory, School of Mechanical Engineering, Beijing Institute of Technology, Beijing 100081, China

Metasurface hologram has emerged as a promising candidate for applications in optical displays, storage and security by exhibiting unprecedented spatial resolution, enormous information capacity and large field of view compared to traditional methods. In order to explore the full capability of the information storage/display and enhance the encryption security of metasurface holograms, smart multiplexing techniques are highly demanded. Here, we integrate multiple polarization manipulation channels for various spatial phase profiles into a single birefringent vectorial hologram by completely avoiding unwanted cross talk. Multiple independent target phase profiles with quantified phase relations, processing significantly different information in different polarization states are realized within a single all-dielectric metasurface. We demonstrate high fidelity, large efficiency, broadband operation, and a total of twelve polarization channels with our metasurface holograms. Such multichannel polarization multiplexing can be used for dynamic vectorial holographic display and provide triple protection to the optical security. The concept is highly promising for applications of arbitrary spin to angular momentum conversion and various phase modulation/beam shaping elements.

O 21.8 Mon 17:45 Poster F

Magensium Nickel Alloy Thin Films for Electrochemical Switching — •Elinor Kath, Florian Sterl, Mario Hentschel, and Harald Giessen — 4. Physikalisches Institut, Universität Stuttgart

Hydrogen can be reversibly loaded in and unloaded from magnesium, which is why magnesium gained significant attention as a potential low-risk storage medium for Hydrogen. Concurrently, magnesium also has found applications in switchable and active plasmonics. While elementary magnesium is metallic, magnesium hydride (MgH_2) is a transparent dielectric which allows switching on and off the plasmonic resonances in individual nanoparticles. For many potential applications the loading and unloading times are impractically long. To increase this switching rate we introduce small amounts of nickel into magnesium films. We are able to fabricate magnesium-nickel alloy thin films with different and controllable nickel concentrations. In our experiments these films are switched gasochromically, that is, using a hydrogen-nitrogen atmosphere, to determine the ideal amount of nickel for the best switching properties. Our measurements show that the loading and unloading times can be significantly reduced in the alloyed systems. Future directions include the potential to switch the magnesium-nickel alloy films electrochemically by immersing them into a KOH electrolyte and applying a negative voltage to the magnesium.

O 22: Overview Talk: Peter Liljeroth

Time: Tuesday 9:30–10:15 Location: H15

Invited Talk O 22.1 Tue 9:30 H15

Engineered electronic states in atomic and molecular lattices — •Peter Liljeroth — Department of Applied Physics, Aalto University School of Science, PO Box 15100, 00076 Aalto, Finland

Constructing designer materials where the atomic geometry and interactions can be precisely controlled is becoming reality. In this tutorial talk, I will discuss the general progress towards this aim using examples based on atomic manipulation by the tip of a scanning tunneling microscope (STM) and molecular self-assembly to reach the desired structures.

Using atomic manipulation, it is possible to construct lattices where every atom is in a well-defined, predetermined position. This opens possibilities for creating artificial materials and I will illustrate this concept by showing how chlorine vacancies on Cu(100) [1] can be used to implement various one- and two-dimensional artificial lattices [2].

Similar concepts can be realized using metal-organic frameworks (MOFs) as a tuneable platform for achieving materials with engineered electronic structures. The synthesis of 2D-MOFs is usually carried out on metal surfaces (e.g. Au, Ag, Cu), where it is difficult to access their intrinsic electronic properties. I will discuss possibilities of synthesizing 2D-MOFs on weakly interacting substrates and assessing their structure and electronic properties through atomic force microscopy (AFM), STM and scanning tunneling spectroscopy (STS) [3].

[1] F.E. Kalff et al. Nat. Nanotech. 11, 926 (2016). [2] R. Drost et al. Nat. Phys. 13, 668 (2017). [3] A. Kumar et al. Nano Lett. 18, 5596 (2018).

O 23: Solid-Liquid Interfaces II: Electrode Surfaces

Time: Tuesday 10:30–13:00 Location: H5

Invited Talk O 23.1 Tue 10:30 H5

Investigating atomic scale structure of liquid metal–electrolyte interfaces — •Bridget M. Murphy — Ruprecht Haensel Laboratory — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

Electrochemical interfaces between immiscible liquids have lately received renewed interest, both for gaining fundamental insight as well as for applications in nanomaterial synthesis. In this contribution, we demonstrate how the atomic scale structure of these previously inaccessible interfaces nowadays is explored by *in situ* synchrotron-based X-ray scattering techniques. Exemplary studies of a prototypical electrochemical system — a liquid mercury electrode in pure NaCl solution — reveal that the liquid metal is terminated by a well-defined atomic layer. This layering decays on length scales of 0.5 nm into the Hg bulk and displays a potential- and temperature-dependent behaviour that can be explained by electrocapillary effects and contributions of the electronic charge distribution on the electrode. In similar studies of nanomaterial growth, performed for the electrochemical deposition of PbFBr, a complex nucleation and growth behaviour is found, involving a crystalline precursor layer prior to the 3D crystal growth. *Operando* X-ray scattering measurements provide detailed data on the processes of nanoscale film formation [1].

[1] B. M. Murphy, S. Festersen, and O. M. Magnussen, Nanoscale, 2016, 8, 13859

O 23.2 Tue 11:00 H5

Resolving the chemical identity of H_2SO_4 derived anions adsorbed on a Pt(111) electrode: they are sulfate. — R. Kramer Campen, Gregor Zwaschka, Igor Ying Zhang, Martin Wolf, and •Yujin Tong — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

One of the model systems in electrochemistry that has been extensively studied is the adsorption of sulfuric acid anions on Pt(111) electrode in acidic solution. While many properties of the adsorbed anion have been well resolved, its chemical nature, whether it is sulfate (${SO_4}^{2-}$) or bisulfate (${HSO_4}^{-}$) is still under debate. The controversy mainly originates from the difficulty in assigning the vibrational mode around 1250 cm^{-1} which has been observed in previous infrared spectroscopic measurements. Here we apply interface-specific, vibrational sum frequency generation (VSF) spectroscopy and theoretical simulation to this problem. By taking advantage of the background-free nature of VSF spectroscopy, we are able to perform more reliable isotope exchange measurements than those done with conventional infrared spectroscopy. The chemical identity of the adsorbate is unambiguously revealed: it is ${SO_4}^{2-}$ rather than ${HSO_4}^{-}$ that adsorbed at the surface even in acidic solution (pH=0), where the dominate solute is essentially HSO_4^-. The distinct different chemical nature of the anion at the surface and in the bulk suggests intriguing interaction between the electrode and the anions.

O 23.3 Tue 11:15 H5

Influence of the polarization of the electrode on the surface plasmon resonance angle shift during adsorption processes on Au(111) — •Karin Schlag, Detlef Nattland, and Rolf Schuster — Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Knowledge about the structure and composition of the double layer is essential for the understanding of electrochemical reactions. We therefore investigated the sulfate adsorption on Au(111) with cyclic voltammetry and in-situ surface plasmon resonance (SPR) spectroscopy. SPR is sensitive to changes of the refractive index at the electrolyte-electrode interface, which is connected to concentration changes of the constituents of the double layer. We observed an increase of the SPR angle during the adsorption process of sulfate on Au(111) by 0.14°.

A multi-layer model based on Abeles' formalism was used to quantify the potential dependent refractive index of the double-layer. We found that the experimentally determined, unexpectedly strong shift of the SPR angle can only partly be explained by the increase of the sulfate concentration at the interface. It is suggested that the polarization of the interface and the subsequent changes of the electron density in the metal surface have to be included in the model.

O 23.4 Tue 11:30 H5

Strain controlled electrocatalysis during Methanol oxidation on gold thin film — •Xinyan Wu[1], Matthias Graf[2,3], and Jörg Weissmüller[1,3] — [1]Institute for Materials Physics and Technology, Hamburg University of Technology, Hamburg — [2]Institute for Electronic and Optical Materials, Hamburg University of Technology, Hamburg — [3]Insitute for Materials Technology, Helmholtz-Zentrum Geesthacht, Geesthacht

It is well known that one method of enhancing the electrocatalytic performance is to tune the surface strain of nanomaterials, by which the adsorption enthalpies could be modified. Based on theories and experiments towards this mechanism, the underlying strain-adsorption-reactivity relationship gradually becomes acknowledged. However, quantifiable experimental observations of the impact of strain for reactivity of catalyst are still rare, which means this field lacks a quantitative experimental database.

Here we exlpore a method, Dynamic Electro-Chemo-Mechanical analysis (DECMA), in order to investigate the impact of elastic strain on the electrocatalystic methanol oxidation reaction on gold thin film surface. In this approach, a sinusoidal strain is applied on the surface of gold electrode during this whole process, and simultaneously the corresponding reaction current and potential signals caused by this known strain are collected through a lock-in technology. In this way, coupling parameters such as potential-strain and current-strain coefficients will be measured and provide effective information for each reaction step.

O 23.5 Tue 11:45 H5

Influence of steps and atomic ensembles for the CO electrooxidation — •Jens Klein, Albert K. Engstfeld, Valeria Chesnyak, Sylvain Brimaud, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The rate of electrocatalytic reactions is often highly sensitive to the surface structure of the metal catalysts.[1,2] To improve the performance of catalyst materials it is inevitable to identify active surface sites and to understand the electrocatalytic processes at the surface sites on an atomic scale.

In this work we report on the role of Pt steps and atomic PtRu ensembles in the CO electro-oxidation i) on Pt(111) model electrodes with varying step density and ii) on Pt_xRu_{1-x}/Ru(0001) surface alloys with varying Pt content, respectively. The model electrodes were prepared and structurally characterized by scanning tunneling microscopy (STM) under ultra-high vacuum (UHV) conditions. The electrocatalytic measurements were performed in an electrochemical flow cell attached to the UHV system. To investigate the role of Pt step sites for the CO electro-oxidation, the steps of the Pt(111) electrodes were passivated for the reaction by condensation of Au. The CO oxidation activity of Pt_xRu_{1-x}/Ru(0001) surface alloys with different Pt contents was correlated with the abundance of specific PtRu ensembles on the surface. We will discuss the influence and importance of defect sites as well as ensemble sites for the electro-catalytic CO oxidation.

[1] M. T. M. Koper, *Nanoscale* **3** (2011) 2054. [2] A. K. Engstfeld et al., *Angew. Chem. Int. Ed.* **53** (2014) 12936.

O 23.6 Tue 12:00 H5

DFT calculations of self-diffusion at an Au(001) electrochemical interface — •Alexandra C. Dávila and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, CAU Kiel, Germany

In surface X-ray scattering experiments at the interface between an Au(100) electrode and $HCl + HAuCl_4$ containing electrolyte Krug et al. [1] have observed that the growth mode depends on the electrode potential and Au-concentration. Transitions from 3D to layer-by-layer and to step-flow growth mode were observed at positive potentials ($V_{Ag/AgCl}$), where the unreconstructed substrate surface is stable. Pichardo-Pedrero et al. [2] have observed an increase of the decay rate of Au islands on Au(001) with sample potential and, in particular, when chloride is present the electrolyte. The atomic-scale mechanism of self-diffusion on coinage metal surfaces has been investigated by DFT calculations before [3, 4], however, the detailed role of the co-adsorbed anions on the diffusion is not yet fully understood. We present diffusion paths on c($\sqrt{2}\times2\sqrt{2}$)R45°-Cl and c(2×2)-Cl Au(001) surfaces. The dependence of the diffusion rate on sample potential as derived from the variation of the induced dipole moment along the paths gives an increase of the Au self-diffusion energy barrier with increasing potential. Thus, we speculate that other factors, like nucleation, determine the sample potential dependence of Au growth mode.

[1] K. Krug *et* al., Phys. Rev. Lett. **96**, 246101 (2006).

[2] E. Pichardo-Pedrero *et* al., Appl. Phys. A, **87**, 461 (2007).

[3] J. E. Müller *et* al., Phys. Rev. B **74**, 085408 (2006).

[4] M. Mesgar *et* al., ChemPhysChem **14**, 233 (2013).

O 23.7 Tue 12:15 H5

Investigation of ion mobility and material transport on KBr surfaces in air in dependence of the relative humidity. — Dominik Kirpal, Korbinian Pürckhauer und •Franz Giessibl — University of Regensburg, Regensburg, Germany

On every surface exposed to humid air a thin film of water molecules forms. The presence of water plays an important role for chemical reactions, material exchange and movement. The effect of condensed water layer, present in ambient conditions plays a significant role especially on surfaces that dissolve easily in water [1]. Surface atoms can easily diffuse into the thin water layer and, when surface conditions are favourable, they can re-attach to the surface. We collected FM-AFM images of the KBr surface in a climate-controlled glove box at various values of relative humidity. By scratching the surface with the AFM tip, we construct energetically unfavourable hills and scratch sites. We observe the time evolution of these sites. We propose that there is a critical value around 25% relative humidity, under which dissolution and reattachment occurs relatively slowly, in contrast to our observations at 28% relative humidity where these processes occur quickly.

[1] M. Luna, et al., Journal of Physical Chemistry A, 102.34 (1998) 6793-6800.

O 23.8 Tue 12:30 H5

Boosting the Scalability of Car-Parrinello Molecular Dynamics for Large-Scale Simulations of Solid-Liquid Interfaces — •Tobias Klöffel[1], Pawel Rodziewicz[2], Gerald Mathias[3], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Department of Chemistry, Jan Kochanowski University, Kielce, Poland — [3]Leibnitz Supercomputing Centre (LRZ), Garching

We present our recent optimizations of the ultra-soft pseudo-potential (USPP) code path of the *ab inito* Car-Parrinello molecular dynamics program CPMD (www.cpmd.org). All relevant USPP routines have been revised to fully support hybrid MPI+OpenMP parallelization. For two time-critical routines, namely the multiple distributed 3d FFTs of the electronic states and a key distributed matrix-matrix multiplication, we have implemented hybrid parallel algorithms with overlapping computation and communication. The achievements in performance and scalability are demonstrated on simulations of liquid water with 128 and up to 2048 molecules. Performance evaluation shows gains of up to one order of magnitude and around 50% peak performance on the node level. The improved CPMD code has been applied to sample the free energy landscape for a hydrolysis reaction in explicit liquid water on a ZnO surface as catalyst. The unit cell contained 735 atoms and 3332 electrons. A 50 ps trajectory required about 10 days on 18 SuperMUC2 compute nodes.

O 23.9 Tue 12:45 H5

The nanoscopic structure of Pt-water electrified interface under bias revealed — •Clotilde Cucinotta — Imperial College

London

In this talk I will introduce some issues connected with the simulation of electrified interfaces at the nanoscale focusing in particular on modelling the effect of an applied potential to an EC cell. I will present some recent progress in the simulation of the double layer of the fundamental Pt-water interface and its response to changes of potential applied to the cell. I will show that the metal/surface charging cannot be described using a traditional simple capacitor model and that the double layer nanoscopic structure, mass density and charge distribution, strongly depend on the applied potential.

O 24: Plasmonics & Nanooptics I: Metastructures and Novel Techniques (joint session O/CPP)

Time: Tuesday 10:30–12:45 Location: H8

O 24.1 Tue 10:30 H8

Creating functional plasmonic fields with orbital angular momentum via meta structures — •Eva Prinz[1,2], Grisha Spektor[3], Michael Hartelt[1], Anna-Katharina Mahro[1], Meir Orenstein[3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany — [3]Department of Electrical Engineering, Technion - Israel Institute of Technology, Israel

Optical fields can carry spin angular momentum (SAM) in the form of circularly polarized light and orbital angular momentum (OAM) as helical wavefronts. In the field of plasmonics, surface plasmon polaritons (SPPs) can carry surface confined OAM in the form of plasmonic vortices. Controlling such vortices opens the door towards a variety of applications.

Plasmonic OAM can be generated by the use of plasmonic vortex lenses (PVLs), a type of coupling structure based on Archimedean spirals. We demonstrate both experimentally and in simulations a modular plasmonic lens assembling strategy for the sculpturing of functional plasmonic fields. This approach is based on meta structures and allows the creation of lenses with an effective chirality that depends on the illumination. The coupling structures are milled into a gold surface and the created SPPs are detected via time-resolved PEEM.

O 24.2 Tue 10:45 H8

Advanced optical programming of individual meta-atoms beyond the effective medium approach — •Andreas F. Hessler[1], Ann-Katrin U. Michel[1], Sebastian Meyer[1,2], Julian Pries[1], Yuan Yu[1], Martin Lewin[1], Tobias W. W. Mass[1], Matthias Wuttig[1], Dmitry N. Chigrin[1,2], and Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen — [2]DWI - Leibniz Institute for Interactive Materials, Aachen

Despite their nanometer thickness, active metasurfaces (MSs) based on phase-change materials (PCMs) enable compact photonic components, offering adjustable functionality for the manipulation of light, such as polarization filtering, lensing and beam steering[1]. Commonly, they feature multiple operation states by switching the whole PCM fully between two states of drastically different optical properties[2]. Intermediate states of the PCM have also been exploited to obtain gradual resonance shifts which are usually uniform over the whole MS and described by effective medium theory. We now demonstrate simultaneous control of size, position and crystallization depth of the switched PCM volume within each meta-atom. By modifying the local optical properties, reflection amplitude and phase can be programmed at the meta-atom scale. This goes beyond previous effective medium concepts and should allow for multiple complex functionalities on the same MS or small adaptive corrections to external aberrations and fabrication errors.

[1] X. Yin et al., Light Sci Appl. 6, e17016 (2017).

[2] M. Wuttig et al., Nat. Photon. 11, 465 (2017).

O 24.3 Tue 11:00 H8

A Spin-Optical Nano Device — •Enno Krauss[1], Gary Razinskas[1], Dominik Köck[1], Swen Grossmann[1], and Bert Hecht[1,2] — [1]Nano-Optics and Biophotonics Group, Department of Experimental Physics 5, University of Würzburg, Würzburg, Germany — [2]Wilhelm-Conrad-Röntgen-Center for Complex Material Systems (RCCM), University of Würzburg, Würzburg, Germany

The photon spin is an important resource for quantum information processing as is the electron spin in spintronics. However, for subwavelength confined optical excitations, polarisation as a global property of a mode cannot be defined. Here, we show that any polarisation state of a plane-wave photon can reversibly be mapped to a pseudo-spin embodied by the two fundamental modes of a subwavelength plasmonic two-wire transmission line. We design a device in which this pseudo-spin evolves in a well-defined way throughout the device reminiscent of the evolution of photon polarisation in a birefringent medium and the behaviour of electron spins in the channel of a spin field-effect transistor. The significance of this pseudo spin is enriched by the fact that it is subject to spin-orbit locking. Combined with optically active materials to exert external control over the pseudo-spin precession, our findings could enable spin-optical transistors, i.e. the routing and processing of quantum information with light on a subwavelength scale.

O 24.4 Tue 11:15 H8

Magneto-optical thermal Hall effect — •Annika Ott[1], Philippe Ben-Abdallah[2], and Svend-Age Biehs[1] — [1]Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany — [2]Laboratoire Charles Fabry, UMR 8501, Institut d'Optique, CNRS, Université Paris-Sud 11, 2, Avenue Augustin Fresnel, 91127 Palaiseau Cedex, France

The control of heat flux at the nanoscale by means of external magnetic fields has attracted much attention, recently. It could be shown that the near-field heat transfer between two magneto-optical slabs can be tuned by the external field [1], and unexpected and very interesting effects like the thermal radiative Hall effect, persistent currents, and giant magneto-resistance [2, 3, 4, 5] have been highlighted. Here we discuss the existence of a circular heat flux [6] as the origin of the thermal radiative Hall effect.

References:

1. E. Moncada-Villa, V. Fernandez-Hurtado, F. J. Garcia-Vidal, A. Garcia-Martin, and J. C.Cuevas, Phys. Rev. B 92, 125418 (2015). 2. P. Ben-Abdallah, Phys. Rev. Lett. 116, 084301, (2016). 3. L. Zhu and S. Fan, Phys. Rev. Lett. 117, 134303 (2016). 4. I. Latella and P. Ben-Abdallah, Phys. Rev. Lett. 118, 173902, (2017). 5. R. M. Abraham Ekeroth, P. Ben-Abdallah, J.C. Cuevas and A. Garcia Martin, ACS Photonics, 5, 705-710, (2018). 6. A. Ott, P. Ben-Abdallah, S.-A. Biehs, Physical Review B, 97, 205414 (2018).

O 24.5 Tue 11:30 H8

Electroluminescence from transparent graphene nanojunctions — •Christian Ott, Martin Hauck, Sascha Korn, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstr. 7/Bau A3, D-91058 Erlangen, Germany

Electroluminescence (EL) emitted from metal-metal tunnel junctions has already been observed in STM experiments in the late 80s [1], nevertheless its origin is still under scientific discussion and is usually attributed either to plasmonic modes triggered by the granular nature of current [2] or to blackbody-like radiation of the injected hot electrons [3]. We report on EL emitted from graphene-graphene nanojunctions (GNJ) fabricated from epitaxial graphene on silicon carbide [4]. In stark contrast to STM experiments, GNJs provide a flat, accessible and transparent geometry, allowing an unobscured optical and electron-microscopic access. The observed EL shows a blackbody like spectrum with surprisingly high apparent temperatures well above the damage threshold of the material. Our findings are critically discussed in terms of differences and similarities to other reported experiments (especially STM) to highlight their contribution to the understanding of an elementary process of light-matter interaction.

[1] Schlittler et al., Z. Phys. B. 72, 497 - 501 (1988) [2] Peters et al., PRL 119, 066803 (2017) [3] Downes et al., Applied Physics Letters 81, 7 (2002) [4] Ullmann et al., Nano Letters 14, 5 (2015)

O 24.6 Tue 11:45 H8

Towards Niobium Plasmonics for Single Photon Detection

— •Ahmed Farag, Monika Ubl, Annika Konzelmann, Mario Hentschel, and Harald Giessen — 4th Physics Institute, Center for Integrated Quantum Science and Technology IQST, and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

With the fast development in single photon based technologies such as quantum computing and quantum cryptography, conventional avalanche photodiodes as single photon detectors are not the optimum tools anymore. They are currently replaced by Superconducting Nanowire Single Photon Detectors (SNSPDs) based on the superconductivity of certain materials. The current challenge with SNSPDs lies in overcoming the trade-off between the detection efficiency and the recovery time. While a large active area will lead to high detection efficiency, the associated high kinetic inductance causes a long recovery time. Plasmonic nanoantennas can play an important role in the absorption enhancement of SNSPDs. These nanostructures provide a high absorption cross section at resonance, significantly larger than their geometric cross section. We present a plasmonic photon detector based on niobium, as one of the common superconductors with low kinetic inductance. Additionally, we are increasing the absorption of our nanostructures even further using the perfect absorber scheme. We fabricated a plasmonic perfect absorber SNSPD, investigated its response to external light at resonance, and proved the plasmonic-based working principle as evidenced by its polarization dependence.

O 24.7 Tue 12:00 H8

Probing surface plasmon with phase-shaped electron energy-loss spectroscopy — •Hugo Lourenco-Martins[1], Davy Gérard[2], Jo Verbeeck[3], Giulio Guzzinati[3], and Mathieu Kociak[1] — [1]Laboratoire de Physique des Solides, Université Paris-Saclay, France — [2]L2n, Université de Technologie de Troyes, France — [3]EMAT, University of Antwerp, Belgium

Electron energy loss spectroscopy (EELS) has attracted a large interest due to its efficiency in resolving plasmonic resonance at the nanometer scale. However, it remained intrinsically unable to detect plasmonic phase-related properties. Nevertheless, vortex electron states constitute a perfect candidate to overcome this limitation and measure optical dichroism in an electron microscope [1]. Moreover, it has been recently demonstrated that such probes can be created in an electron microscope by tailoring the phase of the beam [2]. In the present work [3], we developed a semiclassical formalism describing the interaction between an electron probe with an arbitrary phase profile and a plasmonic mode. We showed that the equation ruling this interaction takes the elegant form of a transition matrix between two electron states mediated by the eigenpotentials of the plasmon modes. In this contribution, we will present the theoretical formalism and a wide variety of numerical studies of interactions between different nano-structures and phase-shaped electron probes, with a special emphasis on the experimental feasibility of the proposed geometries. [1] Asenjo-Garcia et al. PRL 113 (2014) [2] Verbeeck et al, Nature 467 (2010) [3] Guzzinati et al., Nature Com. 8 (2017)

O 24.8 Tue 12:15 H8

Quantitative phase imaging of plasmonic metasurfaces — •Vlastimil Křápek[1], Petr Dvořák[1], Alexander Fassbender[2], Petr Bouchal[1], Martin Hrtoň[1], Jiří Babocký[1], Filip Ligmajer[1], Radim Chmelík[1], Stefan Linden[2], and Tomáš Šikola[1] — [1]Central European Institute of Technology, Brno University of Technology, Purkyňova 123, 612 00 Brno, Czech Republic — [2]Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

We report on wide-field quantitative phase imaging of plasmonic metasurfaces by coherence-controlled holographic microscopy [1] and 4th generation quantitative optical microscopy. Both resonant [2] and geometric phase [3,4] are retrieved for various metasurfaces including a lens and a vortex beam plate. Three-dimensional imaging, polarization sensitivity, and sensitivity down to single antenna is demonstrated.
[1] P. Kolman et al., Opt. Express 18, 21990 (2010).
[2] J. Babocký et al., ACS Photonics 4, 1389 (2017).
[3] A. Faßbender et al., APL Photonics 3, 110803 (2018).
[4] P. Bouchal et al., arXiv 1811.01561.

O 24.9 Tue 12:30 H8

Influence of laser parameters on spatially periodic heating of metals induced by surface plasmon polaritons — •Pavel N. Terekhin[1,2], Pascal D. Ndione[1], Sebastian T. Weber[1], and Baerbel Rethfeld[1] — [1]Department of Physics and Research Center Optimas, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]National Research Centre "Kurchatov Institute", Kurchatov Sq. 1, 123182 Moscow, Russia

We present a detailed investigation of periodic heating of metals and periodic structure formation on their surfaces induced by surface plasmon polaritons (SPPs) after irradiation with ultrashort laser pulses. The interference of the incident and the SPPs electromagnetic waves leads to an enhancement of the resulting field and, therefore, a spatial modulation of the deposited laser energy.

Our aim is to show the influence of laser parameters on the formation of surface structures. The two-temperature model (TTM) is used to calculate the evolution of electronic and lattice temperatures. A new source term in the TTM, which takes into account plasmonic subsystem, is derived. The results obtained indicate that the electronic temperature shows the same spatial oscillations as the source term. Further, these oscillations are still present in the lattice temperature when being heated to the melting point. That could cause the formation of the periodic structures on the surface of the solid. Therefore, the developed model allows calculating materials' heating after ultrashort laser irradiation and studying the fundamental mechanisms of laser energy absorption under controlled conditions.

O 25: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge III (joint session O/CPP/DS/TT)

Time: Tuesday 10:30–13:00 Location: H9

Topical Talk O 25.1 Tue 10:30 H9

Addressing the structure and dynamics of weakly-bonded interfaces — •Mariana Rossi — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin

Interfaces between different materials constitute the basis of technological devices. Incorporating organic components within different architectures opens the path for creating more versatile interfaces with a wide range of properties at a reduced cost. However, the large conformational space that organic components can explore at finite temperatures and the inherent anharmonicity of their intra and intermolecular interactions brings further challenges to first-principles simulations. In this talk, I will discuss our recent efforts to address these challenges, based on developments within density functional theory an ab initio (path integral) molecular dynamics. I will present strategies for conformational space sampling of organic/inorganic interfaces, discuss the relationship between atomic and electronic structure including the effect of different functionals, present techniques to include anharmonicity in vibrational fingerprints and machine learning tools to calculate these at reduced costs, and our recent methodological developments that allow the inclusion of quantum nuclear effects in high-dimensional systems (especially weakly bonded interfaces) using path integral molecular dynamics.

O 25.2 Tue 11:00 H9

Elucidating the Nuclear Quantum Dynamics of Intramolecular Double Hydrogen Transfer in Porphycene — •Yair Litman[1], Jeremy O. Richardson[2], Takashi Kumagai[1], and Mariana Rossi[1] — [1]Fritz Haber Insitute of the Max Planck Society, Berlin, Germany — [2]ETH, Zurich, Switzerland

We address the double hydrogen transfer (DHT) dynamics of the porphycene molecule: A complex paradigmatic system where the making and breaking of H-bonds in a highly anharmonic potential energy surface requires a quantum mechanical treatment not only of the electrons but also of the nuclei[1]. We combine density-functional theory calculations, employing hybrid functionals and van der Waals corrections, with recently proposed and optimized path-integral ring-polymer methods for the calculation of vibrational spectra and reaction rates. Our simulations predict the position and width of the N-H stretching band of porphycene and DHT rates in excellent agreement with experiments, thus confirming our determination of the tunneling pathways and the anharmonic mode couplings that play a role in this reaction. They also provide quantitative information about the usually ignored competition between concerted and stepwise DHT pathways at different temperature. These results show that our theoretical approach can describe hydrogen transfer dynamics in different environments, for example when porphycenes are adsorbed on surfaces in prototype molecular switch architectures[2]. [1] Y. Litman, Richardson, J. O., Kumagai, T., Rossi, M. *arXiv*:1810.05681. [2] T. Kumagai, et al., *J. Chem. Phys.,* **148,** 102330 (2018).

O 25.3 Tue 11:15 H9

Interplay of quantum nuclear fluctuations and the electronic structure of the cyclohexane/Rh(111) interface — •Karen Fidanyan and Mariana Rossi — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, Berlin

Cyclohexane (C_6H_{12}) adsorbed on metal surfaces can participate in catalytic dehydrogenation reactions, which show good potential for hydrogen storage. It has been observed experimentally that C_6H_{12} adsorbed on the Rh(111) surface shows an isotope effect on the work function change and the adsorption energy upon deuteration [1]. The physical origin of this puzzling isotope effect on the electronic structure has not been fully resolved. We employ density-functional theory (PBE functional with van der Waals corrections) and *ab initio* path-integral molecular dynamics at 150 K to characterize the underlying physics of this phenomenon. We perform these simulations almost at classical-nuclei cost by making use of the spatially-localized ring-polymer contraction scheme proposed in Ref. [2]. The harmonic approximation to zero-point-energy in the adsorption energy is not able to capture the isotope effects observed experimentally. We thus include anharmonic corrections through the dynamics and identify the temperature-dependent electronic level broadening and renormalization due to the interaction with phonons in this system.
[1] T. Koitaya and J. Yoshinobu, *Chem. Rec.* **14** 848-856 (2014).
[2] Y. Litman, D. Donadio, M. Ceriotti and M. Rossi, *J. Chem. Phys.* **148** 102320 (2018).

O 25.4 Tue 11:30 H9

Quantum-Nuclear Effects in Anharmonic Thermal Transport of Organic Materials — •Hagen-Henrik Kowalski, Mariana Rossi, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

To date, an accurate computational assessment of thermal transport in organic compounds still constitutes a considerable challenge for first principles theory, since the vibrations in such compounds are to a large extent governed by quantum-nuclear (QN) ***and*** strongly anharmonic (SA) effects [1]. Perturbative approaches account for QN, but not for SA effects, whereas Molecular Dynamics (MD) approaches [2] with classical nuclei account for SA, but neglect QN effects. To overcome this limitation, we here present a framework capable of accounting for both QN and SA effects by sampling the vibrational motion via Thermostatted Ring Polymer Molecular Dynamics (TRPMD). The lattice thermal conductivity is assessed through the Green-Kubo formalism and the auto-correlation of the heat flux. To obtain this quantity, we extend the *ab initio* heat-flux definition proposed in Ref. [2] from MD to TRPMD, in order to include QN effects. We critically discuss the approach, its accuracy, and numerical cost for several materials, ranging from toy-models, e.g., solid Argon, to recently discussed organic materials, in which both QN and SA effects are non-negligible.
[1] M. Rossi, P. Gasparotto, M. Ceriotti, *Phys. Rev. Lett.* **117**, 115702, (2016).
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901, (2017).

O 25.5 Tue 11:45 H9

Electronic Conduction in Metal Junctions with Multi-Heme Proteins — •Zdenek Futera[1], Xiuyun Jiang[1], Jan Elsner[2], and Jochen Blumberger[1,3] — [1]Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom — [2]University of Cambridge, Robinson College, Grange Road, Cambridge CB3 9AN, United Kingdom — [3]Institute for Advanced Study, Technische Universität München, Lichtenbergstrasse 2 a, D-85748, Garching, Germany

Multi-heme proteins such as STC or MtrF are membrane proteins facilitating long-range electron transfer (ET) across cell membrane in metal-reducing bacteria. We have used classical molecular dynamics (MD) together with electronic-structure calculations based on density functional theory (DFT) to show that in native environment the conducted electrons are transferred by incoherent hopping between the heme cofactors. However, recent experimental measurements of current-voltage (I-V) curves suggested that the ET mechanism changes to coherent electron tunneling in vacuum when the protein is electronically coupled with metal electrodes. To investigate such conditions, we performed MD simulations in accurate gold/protein interaction force field to identify adsorption of STC and MtrF between two gold electrodes. By large-scale DFT calculations of the whole interfacial structure we identified the conduction channels formed predominantly by delocalized heme iron states. Finally, we apply Landauer formalism to compute I-V curves on STC junction using the DFT electronic states corrected for band alignment and discuss the ET mechanism.

O 25.6 Tue 12:00 H9

Elastic and lattice-dynamical properties of titanium-based compounds — •Peter Weber, Pasquale Pavone, and Claudia Draxl — Humboldt-Univeristät zu Berlin, Physics Department and IRIS Adlershof, Germany

Titanium is the basic element of a variety of compounds with very different electronic, mechanical, and thermal properties. While, for instance, the rocksalt crystals TiC and TiN are well known for their hardness, allotropes of TiO_2 show much softer elastic behaviour. In this work we present the results of an *ab-initio* investigation of the elastic and lattice-dynamical properties of these compounds under pressure. The elastic-constant tensor is calculated up to the third order. Pressure effects on the lattice-dynamical properties of these compounds are evaluated in terms of the mode Grüneisen parameter at the Brillouin zone center. The calculations are performed using density-functional theory as implemented in the full-potential all-electron software package `exciting` [1]. Linear and nonlinear elastic constants are obtained using the `ElaStic` tool [2].

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202
[2] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184** 1861 (2013)

O 25.7 Tue 12:15 H9

Understanding the electron transport through $NiSi_2$-Si interfaces — •Florian Fuchs[1,2,3,4], Sibylle Gemming[1,2,3], and Jörg Schuster[2,4] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Dresden, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [4]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Metal-semiconductor interfaces are of huge importance for applications and can be found in various field-effect transistors. We study the interface between $NiSi_2$ and silicon on the basis of density functional theory and the NEGF formalism. Different crystal orientations and strain states are investigated systematically.

We focus on the tunneling phenomena of carriers through the Schottky contact at the interface, which are crucial for the on-current in transistors. The on-current is found to be strongly dependent on strain and orientation. It will be shown that the height of the Schottky barrier determines the tunneling current. However, not all changes in the current can be traced back to the barrier height. The modification of the electronic structure matter as well, which can be modeled based on the effective mass of the tunneling carriers. We have also extracted work functions of the isolated materials which we relate to the extracted Schottky barrier heights. It will be shown that the Schottky-Mott model fails for this material system. Better approaches will be discussed in our contribution.

O 25.8 Tue 12:30 H9

Impact of Lattice Screening on Wannier-Mott Excitons — •Claudia Rödl — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Optical properties of materials are most relevant for a large variety of technological applications, ranging from photovoltaics over various spectroscopy techniques to LEDs and displays. In optical spectra, microscopic quantum many-body effects like excitons, i.e. coupled electron-hole-pair excitations, are measurable at a macroscopic scale and crucially determine the materials properties. Hence, a deep understanding of exciton physics constitutes an indispensable driving force for innovation in optics and optoelectronics.

The state-of-the-art parameter-free theoretical description of excitons is based on the Bethe-Salpeter equation of many-body perturbation theory. The present theoretical standard approach takes only the static electronic screening of the electron-hole-pair interaction into account. The coupling of excitons to phonons and, hence, polaronic screening contributions are omitted. However, the exciton-phonon coupling is crucial for the qualitative and quantitative understanding of exciton spectra in materials with strong polaronic effects, such as many technologically highly relevant oxides. We will tackle this problem and explore routes towards the inclusion of the polaronic screening contributions into the Bethe-Salpeter framework. As test systems, we study simple two-atomic bulk semiconductors and insulators.

O 25.9 Tue 12:45 H9

Discovering a novel nanometric cubic phase in monochalcogenide semiconductors - Theory meets experiment — •Guy Makov[1,2], Uri Argaman[1], Elad Segev[2], Ran Abutbul[1,2], and Yuval Golan[1,2] — [1]Dept. of Materials, Ben-Gurion University, Beer-Sheva, Israel — [2]Ilse Katz Institute of nanoscience, Ben-Gurion University, Beer-Sheva, Israel

A new nanometric cubic binary phase with a low-symmetry 64-atom cubic structure was recently discovered in tin monosulfide. Subsequently, this phase was synthesized and identified in tin monoselenide and posited to exist in germanium monosulfide and monoselenide based on density functional theory total energy calculations. A series of computational and experimental studies have identified promising optical properties due to the larger bandgap and non-centrosymmetric structure of the crystal. The structure, atomic positions, band gaps and vibrational spectra of these phases were determined by ab-initio density functional calculations and found to be in very good agreement with experimental measurements. The phases were determined to be mechanically stable from ab-initio phonon spectra and energetically close to competing structures such as rhombohedral and orthorhombic. Surface energy calculations indicate that the particles must be stabilized by ligand adsorption. Ligand surface properties are explored to explain the nanocrystal growth mechanisms. This talk will focus on the results of our calculations on surface and bulk properties and their interplay with experimental studies.

O 26: Focus Session: Designer Quantum Systems I (joint session O/TT)

Toy models are simplistic theoretical constructs, meant to capture the basic principles of complex phenomena observed in experiment. Recent amazing advances in condensed matter physics have enabled the reverse, namely the realization of basic theoretical models in well-controlled artificial experimental systems. Such solid state or molecular realizations of models allow us to tune their parameters, thus they may be termed designer quantum systems and can substantially deepen our understanding. Some talks in this session explore the insights offered by the already famous designer quantum systems; others propose or even report new quantum simulators. Moreover, these designer systems are not limited to single-particle physics but extend to many-body phenomena, such as superconducting correlations.

Organizers: Magdalena Marganska and Jascha Repp (University of Regensburg).

Time: Tuesday 10:30–12:45 Location: H15

Invited Talk O 26.1 Tue 10:30 H15

Imaging Electronic Correlations in Twisted Bilayer Graphene — •Stevan Nadj-Perge — California Institute of Technology, Pasadena, CA, USA

Twisted bilayer graphene with a twist angle close to 1° features isolated flat electronic bands that form a strongly correlated electronic system. Here we investigate properties of this system by probing local tunneling density of states using scanning tunneling microscopy and spectroscopy. We show that the flat bands get deformed when they are aligned with the Fermi level using electrostatic gating. Careful characterization of the bands allows us to estimate energy scale of electron-electron interactions. Our results provide basis for microscopic understanding of correlated quantum phases in small angle twisted bilayer graphene.

Invited Talk O 26.2 Tue 11:00 H15

Designing Electronic Quantum Matter: Fabrication and Characterization with Atomic Scale Precision — •Ingmar Swart — Debye Institute for Nanomaterials Science

In a visionary colloquium nearly sixty years ago, Richard Feynman proposed to study complex and elusive quantum systems using more controllable analogues, an approach known as quantum simulation [later published, 1]. Although quantum simulation based on ultracold atoms in optical lattices, nanophotonic systems, trapped ions and superconducting circuits has been very fruitful, electronic quantum simulators have been lacking behind [2].

In this talk, I will demonstrate that electron gases on well-defined metal surfaces form an excellent platform for quantum simulation. By patterning the surface with atomic scale precision using a scanning tunneling microscope, the electrons can be corralled into artificial lattices of nearly any geometry. The same microscope can then be used to measure the local density of states at all positions of interest and to probe the spatial extend and shape of the wave functions. I will show several examples of how we exploit the tunability of this platform. Particular emphasis will be given to our recent efforts to create and study electronic higher-order topological insulators.

References: 1. Richard P. Feynman, International Journal of Theoretical Physics, 21, 467 (1982). 2. Nature Physics Insight on Quantum Simulation, Volume 8 (2012).

O 26.3 Tue 11:30 H15

Characterisation of pure s- and p-orbital bands in electronic honeycomb lattices — •Thomas Gardenier[1], Jette van den Broeke[2], Ingmar Swart[1], Cristiane Morais Smith[2], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht, The Netherlands — [2]Institute for Theoretical Physics, Utrecht, The Netherlands

Honeycomb systems have generated much interest in experimental and theoretical physics due to their interesting band structures. The architypical example of a honeycomb lattice is graphene. The electronic structure of graphene close to the Fermi level can be understood by only considering C 2pz orbitals. Bands due to coupling of sp2 hybrid orbitals are either much higher or lower in energy. It has been shown that in the absence of hybridisation, the band structure of honeycomb lattices features a topologically non-trivial flat band, as well as Dirac cones formed by px and py orbitals.

We patterned a Cu(111) surface with CO molecules to confine the surface state electrons into a honeycomb geometry. By careful tuning of the lattice parameters, we created a honeycomb lattice where s- and p-orbital bands are separated. Scanning tunneling spectroscopy and wavefunction mapping are used to determine the band structure and visualise the electron densities. The results are complemented by theoretical muffin-tin and tight-binding calculations.

O 26.4 Tue 11:45 H15

Constructing a Topological Insulator Atom-by-Atom — •Saoirsé Freeney — Condensed Matter and Interfaces, Princetonplein 1, 3584 CC Utrecht, The Netherlands

In a honeycomb lattice with alternating hopping strengths (Kekulé lattice), a gap in the energy dispersion is opened. Depending on the ratio of hopping parameters and the shape of the boundary, the band structure is either topologically trivial or non-trivial. Using scanning tunnelling microscopy, we realize Kekulé lattices through the coupling of artificial atoms, created by the careful arrangement of electron scatterers (carbon monoxide molecules) on a 2D electron gas (Cu(111) surface state). The electronic properties were probed using scanning tunnelling spectroscopy and differential conductance mapping. We show that the topologically non-trivial lattice features a robust edge state whereas the trivial equivalent does not. The experimental outcomes align well with results from tight binding and muffin tin calculations.

O 26.5 Tue 12:00 H15

Eu-doped NaI scintillators: Point defects and EuI_2 sheets. — •Martin Setvin[1], Manuel Ulreich[1], Igor Sokolovic[1], Michele Reticcioli[3], Lynn Boatner[2], Flora Poelzleitner[1], Cesare Franchini[3], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institute of Applied Physics, TU Wien, Vienna, 1040, Austria — [2]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831, USA — [3]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Vienna, Austria

Activator impurities and their distribution in the host lattice play a key role in scintillation phenomena. A combination of cross-sectional noncontact atomic force microscopy (nc-AFM) and X-ray photoelectron spectroscopy (XPS) was used to study the distribution of Eu^{2+} dopants in a NaI scintillator activated by 3% of EuI_2. Two types of precipitate structures were identified. First, a single-sheet of EuI_2 layered precipitate is a favoured configuration at the surface. Second, precipitates with a cubic crystal structure and a size below 4 nm were found in the bulk material. A surprisingly low concentration of point defects was detected in all of the investigated samples. The relation between the atomic structure and scintillation will be discussed.

The work was supported by the FWF Wittgenstein Prize Z-250.

O 26.6 Tue 12:15 H15

Machine learning the 3D shape of non-planar molecules from AFM images — •Prokop Hapala[1], Fedor Utirev[1], Niko Oinonen[1], Ondřej Krejčí[1], Filippo Federici Canova[1], Benjamin Alldritt[1], Juho Kannala[2], Peter Liljeroth[1], and Adam Foster[1] — [1]Department of Applied Physics, Aalto University — [2]Department of Computer Science, Aalto University

In recent decade Atomic Force Microscopy with tip functionalized by carbon monoxide (CO) provided unique tool to experimentally image sub-molecular details of individual organic molecules [1]. Yet up to now most experiments are limited to flat aromatic molecules, due to difficulties with interpretation of highly distorted images originating from non-planer molecules due to mechanical relaxation of tip or sample. These problems can be partially overcome using a simple mechanical model [2] which can reproduce those distortions, therefore simulate AFM images for given molecular structure. Testing many possible candidate structures is, however, laborious. Instead we attempt to develop automatic tool to conduct inverse task - i.e. to recover molecular structure from given set of AFM images. Preliminary results suggests that convolutional neural network (CNN) [3] trained on simulated AFM images can learn this inverse mapping rather easily. Yet application of the method on real experimental data, and identification of atomic species remains to be a challenge. [1] Gross, L., et al., Science, 325(5944), 1110-1114 (2009). [2] Lecun, Y., et al., Proceedings of the IEEE, 86(11), 2278-2324 (1998). [3] Hapala, et al. PRB, 90(8), 085421 (2014).

O 26.7 Tue 12:30 H15

Spectral Properties of the Herringbone lattice — M. A. Jimenez Herrera[1], O. Dutta[2], A. Iniguez[3], G. Giedke[2,4], and •D. Bercioux[2,4] — [1]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain — [2]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [3]University of the Basque Country, UPV/EHU, Bilbao, Spain — [4]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain

We investigate the spectral properties of a two-dimensional lattice system described by a non-symmorphic symmetry; specifically, we look at the herringbone lattice that is characterised by two glide symmetries. We model the system via a tight-binding model with horizontal and vertical hopping terms. We evaluate the spectrum of the system in the presence of a perpendicular magnetic field: we show how the Hofstadter's butterfly presents characteristics inherited by the honeycomb and square lattice butterflies. Furthermore, we investigate the appearance of edge states in the system when dimerizing the hopping parameters on the horizontal and vertical direction. We analyse the topological properties of these bands in a similar way to the analysis presented for the case of a symmorphic lattice [1]. Finally, we present a possible implementation in terms of CO atoms placed on the top of a Cu(111) surface [2].

[1] F. Liu, & K. Wakabayashi Phys. Rev. Lett. **118**, 076803 (2017). [2] K. K. Gomes, W. Mar, W. Ko, F. Guinea, & H. C. Manoharan Nature, **483**, 306 (2012).

O 27: Metal Oxide Surfaces I: Structure, Epitaxy and Growth

Time: Tuesday 10:30–13:00 Location: H16

O 27.1 Tue 10:30 H16

Surface characterization of single-crystalline $La_{0.8}Sr_{0.2}MnO_3$ films — •Michele Riva, Giada Franceschi, Michael Schmid, and Ulrike Diebold — Institute of Applied Physics, TU Wien, Wiedner Haupstrasse 8-10/E134, 1040, Vienna, Austria

Solid oxide fuel cells are eco-friendly devices that produce energy from chemical reactions. A widespread material for the cathode of such devices is Sr-doped lanthanum manganite ($La_{0.8}Sr_{0.2}MnO_3$, or LSMO). Although the reactions that occur at the LSMO surface during the device operation highly affect its overall efficiency, little to nothing is known about the atomic details of its surface, and how these details affect the ongoing chemical reactions. The scarcity of such investigations is mainly due to the lack of available single crystals. We overcome this limitation by growing high-quality LSMO films by PLD. We characterize the films with a plethora of surface science techniques (STM, LEED, XPS, LEIS), and with *ex-situ* XRD, RBS, TEM, and SMOKE.

Our efforts point to the establishment of a model system for the LSMO surface, while investigating the effect of different growth and preparation conditions. Different growth parameters result in different surface compositions and surface structures, related to each other through a composition phase diagram: Deposition of controlled amounts of MnO, La_2O_3, and SrO allows to move between the different structures in a continuous and reversible way.

O 27.2 Tue 10:45 H16

The surface phase diagram of strontium-lanthanum manganite in STM — •Giada Franceschi, Michele Riva, Michael Schmid, and Ulrike Diebold — Institute of Applied Physics, TU Wien, Wiedner Haupstrasse 8-10/E134, 1040, Vienna, Austria

Solid oxide fuel cells are energy conversion devices that produce clean electricity by electrochemically oxidizing a fuel. This reaction follows the incorporation of oxygen in the device via a cathode surface; the rate of this reaction is limiting the device efficiency. In most commercial applications, the cathode material is Sr-doped lanthanum manganite ($La_{0.8}Sr_{0.2}MnO_3$, or LSMO). Recent studies have demonstrated that the surface atomic details of a related complex oxide, $SrTiO_3$, are key to the oxygen incorporation [1]. To enable similar investigations on the technologically-relevant LSMO, a model for its surface structures needs to be established. To this end, we have combined pulsed laser deposition with surface techniques (most prominently STM), to grow epitaxial crystalline LSMO(110) films (10-100 nm-thick) on $SrTiO_3$(110). We observe a plethora of composition-related surface reconstructions that compensate for the bulk polarity. We will show our current understanding of these surface structures, along with some considerations about their stability under different oxygen chemical potentials.

[1] Riva, *et al.*, Nat. Comm., 9, 3710 (2018)

O 27.3 Tue 11:00 H16

Atomically-resolved AFM study of the bulk-terminated $SrTiO_3$ (001) 1x1 surface — •Igor Sokolović, Michael Schmid, Ulrike Diebold, and Martin Setvin — Institute of Applied Physics, TU Wien, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria

Working with bulk-terminated perovskite surfaces is challenging since the surface preparation techniques suitable for preparation of binary oxide surfaces lead to a plethora of surface reconstructions. We successfully cleaved the prototypical cubic perovskite oxide, $SrTiO_3$ (STO), by utilizing strain-induced ferroelectricity, and possibly found a way to cleave other cubic perovskites with no preferable planes of cleavage. The bulk-terminated (1x1) STO (001) surface was investigated by non-contact atomic force microscopy (ncAFM) which reveals that the as-cleaved surface consists of two distinct terminations: terraces with a metallic TiO_2 and a semiconducting SrO termination, both being up to micrometers in size. During the cleaving Sr atoms are pulled out of the top SrO layer and remain on the opposite TiO_2 surface in the form of adatoms; the concentration of these Sr adatoms is the same as the concentration of Sr vacancies on the SrO surface. These charged point defects serve as a polarity compensation mechanism for stabilizing the strain-induced polarity along the [001] direction in the crystal. Annealing the surface gradually alters the (1x1) termination and turns the surface amorphous.

O 27.4 Tue 11:15 H16

Plasma assisted cleaning and homoepitaxial growth of $\beta-Ga_2O_3$. — •Nicolas Braud, Felix Feske, Thomas Schmidt, and Jens Falta — Institute of Solid State Physics, University of Bremen, Germany

$\beta-Ga_2O_3$ is expected to play an important role in power electronics due to its high breakdown field and high Baliga figure of merit. In addition, gallium oxide has a wide band gap of 4.9 eV, wich enables exciting applications as transparent conducting oxide (TCO).

In this work, annealing in molecular as well as in atomic oxygen have been compared to a sputter-cleaning approach. Optimum results regarding hydroxide and carbon removal, surface morphology and structure has been achieved with plasma assisted cleaning at up to 700 °C, as revealed by x-ray photoelectron spectroscopy, low-energy electron diffraction, and microscopy.

We also present structural and morphological investigations of the initial homoepitaxial growth by molecular beam epitaxy of β-Ga_2O_3 on two different surface orientations: (100-) and (010)-β-Ga_2O_3.

Invited Talk O 27.5 Tue 11:30 H16

Cationic mixing in metal-supported oxide ultra-thin films: interplay of intrinsic and substrate-induced effects — •Jacek Goniakowski and Claudine Noguera — Institut des Nanosciences de Paris, CNRS and Sorbonne Université, Paris, France

Ternary and mixed oxides represent promising materials for many applications because combining cations of different sizes and electronegativities can be used to tune the structural and electronic properties of the resulting oxide alloys. At the nano-scale, these properties are additionally impacted by an interplay of intrinsic (size and dimensionality) and substrate-induced effects. However, despite rapid advances in the fabrication, the characterization, and the control of supported oxide ultra-thin films, a unified conceptual picture of the factors which drive their mixing characteristics at the nano-scale has not yet emerged.

In this context, considering the technological importance of transition metal oxides and in particular of M_2O_3 sesquioxides, we will consider a series of Au-supported MM'O_3 honeycomb monolayers (M, M' = Ti, V, Cr, and Fe) and we will analyse the microscopic mechanisms responsible for the cationic mixing, with the help of first principle calculations. Moreover, we will highlight the nano-oxide nature of such supported monolayers, which distinguishes them from the corresponding unsupported films and bulk materials.

O 27.6 Tue 12:00 H16

identification of two-dimensional FeO_2 termination of hematite $\alpha - Fe_2O_3(0001)$ surface — •Jesús Redondo[1,2], Petr Lazr[3], Pavel Procházka[4], Stanislav Průša[4], Jan Lachnitt[2], Benjamín Mallada[1], Aleš Cahlík[1], Jan Berger[1], Břetislav Šmíd[2], Pavel Jelínek[1], Jan Čechal[4], and Martin Švec[1] — [1]Institute of Physics, Czech Academy of Sciences, Prague — [2]Faculty of Mathematics and Physics, Charles University, Prague — [3]RCPTM, Olomouc — [4]CEITEC, Brno

Iron oxides are among the most abundant compounds on Earth and have consequently been studied and used extensively in industrial processes. Despite these efforts, concrete understanding of some of their surface phase structures has remained elusive, in particular the oxidized $\alpha - Fe_2O_3(0001)$ hematite surface. We detail an optimized recipe to produce this phase over the entire hematite surface and study the geometrical parameters and composition of its complex structure by means of atomically resolved microscopy, electron diffraction and surface-sensitive spectroscopies. We conclude that the oxidized $\alpha - Fe_2O_3(0001)$ surface is terminated by a two-dimensional iron oxide with structure, lattice parameters, and orientation different from the bulk substrate. Using total-energy density functional theory for simulation of a large-scale atomic model, we identify the structure of the surface layer as antiferromagnetic, conductive $1T - FeO_2$ attached on half-metal terminated bulk. The model succeeds in reproducing the characteristic modulations observed in the atomically resolved images and electron diffraction patterns.

O 27.7 Tue 12:15 H16

Surface structure of Ti-doped Hematite α-Fe_2O_3 films grown by pulsed laser deposition — •Florian Kraushofer, Giada Franceschi, Zdenek Jakub, Magdalena Bichler, Michele Riva, Michael Schmid, Ulrike Diebold, Peter Blaha, and Gareth S. Parkinson — TU Wien, Vienna, Austria

Hematite (α-Fe_2O_3) is a promising material for technological applications due to its abundance, low cost, and chemical stability. Its 2.2 eV bandgap makes it potentially ideal as a photoanode for photoelectrochemical water splitting, but performance is hampered by slow reaction kinetics and the need for a significant overpotential.

One widespread strategy for improving the electrocatalytic behavior of hematite anodes is to dope them slightly with titanium. However, the resulting performance usually scales with the doping level in a non-trivial way, suggesting multiple competing effects, such as independent modification of bulk conductivity and surface reactivity. How the hematite surface is modified by the presence of titanium has not been explored in depth.

Here we present an atomic-scale scanning tunneling microscopy (STM) study of Ti-doped hematite films, grown homoepitaxially on undoped hematite single crystals by pulsed laser deposition. We show that on hematite $(1\bar{1}02)$, titanium substitutes iron in the surface layer to form areas of an ilmenite-type $FeTiO_3$ termination even at low bulk doping levels, suggesting preferential agglomeration in the surface. For comparison, titanium was also deposited directly on an undoped hematite sample, which yields the same surface modification after annealing.

O 27.8 Tue 12:30 H16

In-situ growth study of Fe_3O_4/NiO bilayer and $NiFe_2O_4$ films using surface sensitive high energy x-ray diffraction — •Martin Hoppe[1,2], Tobias Pohlmann[1,2], Florian Bertram[2], Jannis Thien[1], Kevin Ruwisch[1], and Joachim Wollschläger[1] — [1]University of Osnabrück, Osnabrück, Germany — [2]DESY, Hamburg, Germany

The (inverse-) spinel structure of ferrites displays a large variety of electronic and magnetic properties[1], making some of them interesting for potential applications in spintronics. The performance of such ferrites as thin film devices, however, is strongly coupled to the structure and interface of these materials, which are determined by the growth conditions.

With the help of surface sensitive High Energy X-Ray Diffraction (HEXRD) it was possible to record several crystal truncation rods and film reflections simultaneously on a large area Detector and achieve a good time resolution within the few seconds range, which has also been shown with CO oxidation on Pd(100) by Gustafson, et al.[2].

In this study, we investigated the growth of Fe_3O_4/NiO bilayers and $NiFe_2O_4$ on both MgO(001) and $SrTiO_3$(001) substrates. By recording simultaneously several CTRs we could follow the evolution the Laue fringes time dependent. By tracing the film peak position as a function of time strain parameters could be extracted as function of film thickness.

[1] *K. Kuepper et al.*, Phys. Rev. B **94.2** (2016), 024401
[2] *J. Gustafson et al.*, Science **343** (2014), 6172 758 – 761

O 27.9 Tue 12:45 H16

Iron cation diffusion in the near-surface region of Fe_3O_4 (001) — •Steffen Tober[1,2], Marcus Creutzburg[1,2], Björn Arndt[1,2], Konstantin Krausert[1,2], Stefan Mattauch[3], Sabine Pütter[3], Amir S. Mohd[3], Alexandros Koutsioubas[3], Lukas Volgger[4], Herbert Hutter[4], Heshmat Noei[1], Vedran Vonk[1], Dieter Lott[5], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-synchrotron Hamburg — [2]Universität Hamburg, Fachbereich Physik — [3]Jülich Centre for Neutron Science — [4]Technische Universität Wien, CTA — [5]Helmholtz Zentrum Geesthacht

Magnetite is a versatile catalyst, used for example in the water-gas-shift-reaction or the Fischer-Tropsch synthesis. Its excellent catalytic properties are closely linked to the defect structure in the near surface region. Scanning tunnelling microscopy (STM) and low energy electron diffraction (LEED) studies of the $(\sqrt{2}\times\sqrt{2})$R45 ° reconstructed (001) surface suggested a subsurface cation vacancy stabilisation mechanism, also confirmed by surface x-ray diffraction (SXRD) [1,2].

We present the results for the homoepitaxial growth of $^{57}Fe_3O_4$ on magnetite (001) substrates by reactive molecular beam epitaxy (MBE). Using ^{57}Fe as a marker, the interdiffusion of iron ions across the film-substrate interface was followed by combining neutron reflectometry [3] and time of flight secondary ion mass spectroscopy (TOF-SIMS).

[1] Bliem, R. et al. Science. 346, 1215 (2014)
[2] Arndt, B. et al. Surf. Sci. 653, 76 (2016)
[3] Schmidt et al., Adv. Eng. Mat. 11, 446 (2009)

O 28: Organic Molecules on Inorganic Substrates I: Switching and Manipulation

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

O 28.1 Tue 10:30 H24

Controllable three-terminal molecular switch based on adsorption site jiggling — •Anja Bauer[1], Markus Maier[2], Josefine Diegel[1], Werner Schosser[1], Fabian Paschke[1], Yuriy Dedkov[1,3], Fabian Pauly[1], Rainer Winter[2], and Mikhail Fonin[1] — [1]Department of Physics, University Konstanz, D-78457 Konstanz — [2]Department of Chemistry, University Konstanz, D-78457 Konstanz — [3]Department of Physics, Shanghai University, 200444 Shanghai, China

Realization schemes for tuning the electronic and magnetic properties as well as for the control of molecular motion on surfaces are of crucial importance for the fabrication of molecule-based functional devices. One possibility to controllably tune the properties of individual molecules relies on the atomically precise manipulation of the environment.

Here, we investigate the switching behavior of single triazatruxene (TAT) molecules on Ag(111) by low temperature STM. Time-dependent current measurements reveal a current-induced telegraph noise, which is characteristic for switching between well-defined states. The pristine TAT molecule switches between three states of different adsorption geometry and orbital population. The switching rate can be efficiently controlled by the tunneling parameters. We further show the possibility to controllably initiate or suppress the switching process by detaching or attaching hydrogen to the nitrogen atoms of TAT as well as to manipulate the switching rates by modification of the molecule's environment.

O 28.2 Tue 10:45 H24

Electrochemistry of single molecules by atom manipulation — •Shadi Fatayer, Florian Albrecht, Nikolaj Moll, Gerhard Meyer, and Leo Gross — IBM Research - Zurich

The charge state of an adsorbed molecule significantly affects its physical as well as its chemical properties, for example, adsorption position, molecular conformation and aromaticity. The proven capabilities of single-electron sensitivity [1,2] and atomic-resolution [3] of atomic force microscopy (AFM) make it an ideal tool to perform charge-state manipulation experiments while atomically resolving the induced changes within the molecule. Here, we present AFM-based results that demonstrate both the control in charge-state and the capability of resolving the atomic structure of a single molecule for different molecules.

[1] L. Gross, et al. Science 324, 5933 (2009) [2] S. Fatayer, et al. Nature Nanotechnology 13, 376 (2018) [3] L. Gross, et al. Science 325, 5944 (2009)

O 28.3 Tue 11:00 H24

Effect of deprotonation on the electronic structure of phthalocyanine molecules on molybdenum disulfide — •Gael Reecht, Nils Krane, Christian Lotze, and Katharina J Franke — Freie Universität Berlin , Berlin ,Germany

Scanning probe techniques (SPM) enable the modification of the chemical structure of single molecules with atomic precision. The formation of radicals is one the capabilities of this single-molecule chemistry but their stabilization is generally inhibited for molecule directly adsorbed on a metal substrate. Here we study by scanning tunneling microscopy and spectroscopy free-base phthalocyanines on MoS_2/Au(111). We observe that under the influence of the tip, the molecule can be modified with major changes of its electronic structure. By investigating the tautomerization properties of the phthalocyanine and with DFT simulations in gas phase, we determine that the modification of the molecule is due to a deprotonation, from H_2Pc to HPc. With the MoS_2 acting as decoupling layer, the deprotonated molecule keep its radical character, with the HOMO being singly occupied.

O 28.4 Tue 11:15 H24

Influence of the spatial extent of molecules on their properties as detectors in MONA applications — •Tim Zenger[1], Jens Kügel[1], Markus Leisegang[1], and Matthias Bode[1,2] — [1]Physikalisches Institut, Experimentelle Physik II, *Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Wilhelm Conrad Röntgen Center of Complex Material Systems (RCCM), *Universität Würzburg, Am Hubland, 97074 Würzburg

The Molecular Nanoprobe (MONA) technique [1] takes advantage of dynamic processes in molecules to enable the measurement of electron transport on a nanometer scale via STM. In this technique charge carriers injected from the STM tip propagate through the sample until they are detected by a molecule, usually phthalocyanine, via a reversible proton transfer reaction, called tautomerization. In contrast to a STM probe, however, these macromolecules possess a significant spatial extent that could have an effect on their properties as detectors of electronic transport. Here we present studies of phthalocyanine molecules to investigate the influence of its cross-like arms on the switching properties in MONA measurements. In detail, we show both angular and distance-dependent measurements of the switching probabilities. These results are compared to naphthalocyanine molecules, which are characterized by larger arms.

[1] M. Leisegang *et al.*, Nano Lett. **18**, 3, 2165-2171 (2018)

O 28.5 Tue 11:30 H24

Controlled consecutive charging of self-assembled clusters of molecules — •Philipp Scheuerer and Jascha Repp — University of Regensburg, Regensburg, Germany

Molecular self-assembly on insulating films [1] or insulators is a promising approach to create functional molecular structures as building blocks for future electronics. Controlled manipulation of single electrons in such structures as recently demonstrated for individual weakly coupled molecules on insulating films [2], represents an important step to understanding intermolecular electronic interactions.

Here, we investigate the charge transfer in self-assembled molecular structures of Perylenetetracarboxylic dianhydride (PTCDA) molecules on thick insulating films. By applying a bias voltage between the tip of a non-contact atomic force microscope and the underlying conductive sample we inject charges into small molecular clusters with single-electron control. Making use of the sensitivity of AFM to detect single electrons we locate the position of charges within clusters. Depending on the number of injected charges either stable charge configurations or tip-induced motion of charges within the island is observed. The latter leads to a damping signal with a pronounced spatial signature.

[1] S. Burke et al., Nature Communications 6, 8312 (2015)
[2] W. Steurer et al., Nature Communications 6, 8353 (2015)

O 28.6 Tue 11:45 H24

Discriminating and counting the possible molecular conformations in a prototypical molecular wire junction — •Marvin Knol[1,2], Alexander Diener[1,2], Philipp Leinen[1,2], F. Stefan Tautz[1,2], and Christian Wagner[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology

Mechanical manipulation of molecules with a scanning probe microscope (SPM) is a versatile technique to study molecular properties and to create new single-molecular devices [1,2,3]. One example is the exciting research field of quantum transport through molecules, which is often hampered by the lack of precise control over the molecular junction conformation. Here we report molecular manipulation experiments in which a single PTCDA (perylene-tetracarboxylic dianhydride) molecule is suspended between two metal electrodes; a Ag(111) surface and a non-contact AFM/STM tip in a variety of discrete junction conformations. We record frequency shift and conductance fingerprints in a tip-space volume of only 0.1 A^3 and perform a statistical analysis thereof to discriminate and count the possible tip-molecule-surface conformations. Our work is a step towards the complete identification of the so-far unobservable atomic structure of molecular junctions and could be the key to fully reproducible quantum transport studies.

[1] C. Wagner et al. Phys. Rev. Lett. 115, 026101 (2015)
[2] T. Esat et al. Nature 558, 573 (2018)
[3] R. Temirov et al. Phys. Rev. Lett. 120, 206801 (2018)

O 28.7 Tue 12:00 H24

Molecular motors studied on surfaces by scanning tunneling microscopy — •Monika Schied[1], Peter Jacobson[1], Dongdong Liu[2], James M. Tour[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, Austria — [2]Department of Chemistry, Rice University, USA

Artificial molecular motors that convert an external energy input into controlled motion have seen great developments in the last decades [1]. While many studies exist in solution, little is known how such functional molecules behave on a surface. Molecules on surfaces have the advantage of a fixed point of reference and confinement in two dimensions making it easier to study the directionality of their motion.

The uni-directional rotation of the motors investigated in this study is based on a combination of double bond isomerisation and helix inversion. This so-called Feringa motor has already been implemented into molecular structures to enable or enhance their lateral translation on metal surfaces [2, 3].

Here, we image single motor molecules on metallic surfaces by low-temperature scanning tunnelling microscopy (STM). To obtain insight into the underlying processes, the same molecule is imaged before and after applying an external stimulus, using either light or voltage pulses from the STM tip, and changes in the molecular adsorption are studied.

[1] W. R. Browne and B. L. Feringa, Nat. Nanotech. 1, 25 (2006)
[2] T. Kudernac et al., Nature 479, 208 (2011)
[3] A. Saywell et al., ACS Nano 10, 10945 (2016)

O 28.8 Tue 12:15 H24

Imprinting Directionality into Proton TransferReactions of an Achiral Molecule — •Markus Leisegang[1], Jens Kügel[1], and Matthias Bode[1,2] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Wilhelm Conrad Röntgen Center of Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg

Molecular motors play a mayor role in biological processes. This has inspired scientists in the past to design molecular machines with controlled functionality on the nanoscale [1]. One key feature of any motor is directional motion. In molecules directional motion is usually induced by structural chirality which on one hand restricts the motion to a fixed direction, but on the other hand can't easily be changed [2]. Here we present a scanning tunneling microscopy study of achiral H_2Pc and HPc molecules that acquire chirality by adsorption onto a Ag(100) surface. The induced chirality is caused by a $-29°$ ($+29°$) rotation of H_2Pc with respect to the [011] substrate direction, resulting in tautomerization that preferentially occurs in a clockwise (counterclockwise) direction. The directionality is found to be independent of energy and location of charge carrier injection. We show that—in contrast to unalterable structural chiralities determined by the molecular structure—the direction of proton motion in HPc on Ag(100) can be inverted by a rotation of the molecule.

[1] M. van den Heuvel *et al.*, Science **317**, 333-336 (2007)
[2] J. Berna *et al.*, Nat. Mater. **4**, 704 (2005)
[3] J. Kügel *et al.*, ACS nano **12**, 8733-8738 (2018)

O 28.9 Tue 12:30 H24

High-Resolution Vibronic Spectra of Molecules on Molybdenum Disulfide Allow for Rotamer Identification — Nils Krane[1], •Christian Lotze[1], Gaël Reecht[1], Lei Zhang[2], Alejandro L. Briseno[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin — [2]Department of Polymer Science and Engineering, University of Massachusetts, USA

Scanning tunneling spectroscopy (STS) is a tool that allows to address individual molecules in a precisely known surrounding. However, it bears the drawback that it requires a conductive substrate. Deposition of organic molecules on a metal substrate leads to strong hybridization of the electronic states. Preservation of the molecular character requires the inclusion of thin band-gapped materials.

Here, we present STS experiments performed on 2,5-bis(3-dodecylthiophen-2-yl)thieno[3,2-b]thiophene (BTTT) molecules adsorbed on a single layer molybdenum disulfide (MoS_2) on Au(111). We show that it acts as an effective electronic decoupling layer that exhibits a small electron-phonon coupling strength. Differential conductance spectra of the molecules exhibit a multitude of sharp characteristic peaks, originating from vibronic states of BTTT. These vibronic fingerprints of different molecules allow for an identification of different rotamers. DFT calculations of the molecule in gas phase provide all details for an accurate simulation of the vibronic spectra of both investigated rotamers [1].

[1] Krane, *et al.*, ACS Nano, 2018, 12, 11, 11698-11703

O 28.10 Tue 12:45 H24

Machine learning for single molecule manipulation — Philipp Leinen[1,2], Malte Esders[3], Kristof Schütt[3], Klaus-Robert Müller[3], F. Stefan Tautz[1,2], and •Christian Wagner[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA Fundamentals of Future Information Technology, Jülich, Germany — [3]Institut für Softwaretechnik und Theoretische Informatik, Technische Universität Berlin, Germany

The controlled mechanical manipulation of individual molecules with a scanning probe microscope (SPM) allows the fabrication of single-molecule devices [1,2] and metastable supramolecular assemblies [3]. Machine learning can reduce the tedious work of finding a successful manipulation protocol for a certain manipulation tasks. We use reinforcement learning (RL) to automatically solve the prototypical task of removing a single PTCDA (perylene-tetracarboxylic dianhydride) molecule from a hydrogen-bonded assembly [3]. Since our RL application is not fully in-silico but receives its feedback from an actual experiment, it needs a training efficiency on par with a human to be useful. We achieve this by teaching the machine some “intuition” about the Cartesian space in which the manipulation takes place by, e.g., spawning a series of weak learners along all tried trajectories and training on unseen state-action pairs. Our method could be a blueprint for solving various manipulation tasks posed in a Cartesian space.

[1] C. Wagner et al. Phys. Rev. Lett. 115, 026101 (2015)
[2] T. Esat et al. Nature 558, 573 (2018)
[3] M. F. B. Green et al. Beilstein J. Nanotechnol. 5, 1926 (2014)

O 29: Nanostructures at Surfaces III: Dots, Particles, and Clusters

Time: Tuesday 10:30–13:00 Location: H25

O 29.1 Tue 10:30 H25

Negative differential resistance in the electron-transport through cuprous oxide thin films — •Alexander Gloystein and Niklas Nilius — Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany

Copper nano-islands grown on Cu2O(111) thin films have been investigated by scanning tunneling microscopy and spectroscopy. The latter reveals pronounced lateral quantization effects in the Cu 4sp states, reflecting the finite island size. Below the onset of the quantized states, a wide region of negative differential resistance (NDR) opens up in the tunneling spectra. The effect is explained with the development of p-type conductance in the Cu2O films below the ad-copper, which promotes electron transport at small negative bias but leads to a sudden closure of transport channels below a critical bias of -1.0 V. The resulting NDR effect exhibits an on/off current that is larger than in common molecular junctions and might qualify this inorganic system for applications.

O 29.2 Tue 10:45 H25

Ultrafast librations of supported nanoclusters studied with femtosecond electron diffraction — •Thomas Vasileiadis[1], Emmanuel Skountzos[2], Dawn Foster[3], Shawn Coleman[4], Daniela Zahn[1], Vlasis Mavrantzas[2], Richard Palmer[5], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin, Germany — [2]Department of Chemical Engineering, University of Patras — [3]Nanoscale Physics Research Laboratory, School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham B15 2TT, United Kingdom — [4]US Army Research Laboratory, Weapons and Materials Research Directorate — [5]College of Engineering, Swansea University, Bay Campus, Fabian Way, Swansea SA1 8EN, United Kingdom

Femtosecond electron diffraction (FED) [1] can be used to probe ultrafast atomic motions in laser-excited bulk solids and nanoscale heterostructures [2]. In this work we show that, due to the sensitivity of diffraction in the crystal orientation, FED is sensitive to rotations of nanoclusters on a membrane. The investigated samples are size-selected Au nanoclusters with a partial (111) orientation on few-layer graphite. Optical excitation brings the nanoclusters and the substrate in non-equilibrium conditions. Due to substrate phonons, Au NCs perform ultrafast, constrained rotations, termed librations, which change the relative intensities of the various diffraction peaks in the picosecond timescale. References: [1] Waldecker et al. JAP 117, 044903 (2015). [2] Vasileiadis et al. ACS Nano 12 (8),7710-7720 (2018).

O 29.3 Tue 11:00 H25

Virtual Plasmonic Dimers of Silver Nanoparticles on Si(111)-(7x7) unraveled by Size-Correlated Single-Object Photoemission — •Kevin Oldenburg[1], Hannes Hartmann[1], Jean Lermé[2], Karl-Heinz Meiwes-Broer[1], Sylvia Speller[1], and Ingo Barke[1] — [1]University of Rostock, Institute of Physics, 18059 Rostock, Germany — [2]Université de Lyon, Institut Lumière Matière, 69622 Villeurbanne Cedex, France

Single object spectroscopy is capable of unravelling individual features of clusters at surfaces. Here we show that for highly polarizable substrates the frequently applied picture of an "effective" dielectric medium surrounding each particle falls short due to coupling of the particle plasmon with its image dipole [1,2]. Silver nanoparticles deposited on Si(111)-(7x7) are investigated by using PEEM, thus probing a large number of particles simultaneously. We show that even for sizes as small as 10 nm the dipole approximation breaks down, because the system inherently creates higher-order multipole modes [3]. Model calculations based on Generalized Mie theory [2] reveal that the formation of multipole modes is extremely sensitive to the local geometry on the scale of one Angström, expressed by the effective intra-dimer separation. On the one hand this leads to a fundamentally limited control over particle plasmon energies. On the other hand selective excitation enables tailored energy transfer into molecular aggregates by utilizing certain metal nanoparticles as nanoscopic light sources.

[1] Knight et al., Nano Letters 9, 2188 (2009) [2] Lermé et al., J. Phys. Chem. C 117, 6383 (2013) [3] Oldenburg et al., under review

O 29.4 Tue 11:15 H25

In-situ monitoring of nanoparticle generation in plasma — •Oleksandr Polonskyi, Jonas Drewes, Alexander Vahl, Thomas Strunskus, and Franz Faupel — Chair for Multicomponent Materials, Faculty of Engineering, Kiel University, Germany

The unique properties of nanoparticles (NPs) associated with their dimensions make them very attractive for the growing field of nanotechnology. The methods of their synthesis allowing a simple and reliable tuning of NP dimensions as well as chemical structure are in a high demand. Here, we focus on a plasma based approach for generation of metallic NPs utilizing a magnetron sputtering operating at a relatively high gas pressure (˜100 Pa). This method become very attractive for NP generation providing the ability to deposit various types of NPs with good control over size and size distribution. However, the processes during NP formation in plasma are not fully understood yet and require more advanced in-situ methods to follow NP growth. Here we report on the investigation of the initial stages of metallic NP growth in a gas phase by broadband transmission UV-Vis spectroscopy. We demonstrate that due to their strong particle plasmon resonance, small clusters and NPs can be monitored by UV-Vis spectroscopy in-situ during growth and transport. We found that small clusters are already generated in the region close to the magnetron target surface. Our measurements indicate that a high concentration of nanoparticles is located near the magnetron because of trapping in a plasma volume.

O 29.5 Tue 11:30 H25

Elucidating morphology changes in MgO supported Palladium nanoparticles — •Jan-Christian Schober[1,2], Simon Chung[1], Vedran Vonk[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronensynchrotron Hamburg — [2]Universität Hamburg, Fachbereich Physik

Noble metals are of great importance in heterogeneous catalysis of CO oxidation and NO_x reduction. While already existing practical applications usually consist of oxide supported nanoparticles, oxidation behaviour and the precise catalytic processes occuring are still not completely understood on the atomic scale.

It was shown that at elevated temperature and in oxygen atmosphere palladium nanoparticles undergo a reversible shape change [1], however the time-scale and energetics of this process are still unknown. We aim to build on the results of this study and elucidate the formation and diminishing of the {112} facets in oxygen atmospheres ranging from ultra-high-vacuum to 1 bar and temperatures from 300 K to 900 K in order to establish a phase diagram of the particle morphology.

Observing the intensity of the {111} and {112} facet in a diffraction experiment allows to determine the conditions at which the phase change occurs as well as the relative size of the facets.

[1] P. Nolte *et al.*, Nano Lett. **1**, 4697-4700 (2011)

O 29.6 Tue 11:45 H25

Understanding charge transfer and electronic polarization of Au nano-catalysts supported on reduced TiO_2(110) surfaces — •Su-Hyun Yoo[1], Niklas Siemer[2], Mira Todorova[1], Dominik Marx[2], and Jörg Neugebauer[1] — [1]Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Lehrstuhl für Theoretische Chemie, Ruhr Universität Bochum, 44780 Bochum, Germany

Gold nanoparticles on TiO_2(110) surfaces containing oxygen vacancies are of great interest due to their catalytic activity respective oxidation reactions, such as the water gas shift reaction, the CO oxidation reaction and others. Despite extensive studies, the nature of the interactions between oxygen vacancy, substrate and the gold nanoparticle remains controversial, which hampers an understanding of the catalytic mechanism. Combining ab-initio molecular dynamics calculations with methods developed in semiconductor physics to study defects, we investigate the interactions between the vacancy and the nanoparticle for a representative set of density-functionals theory (DFT) exchange-correlation functionals (PBE, PBE+U and two hybrid functionals). The obtained band diagrams allow us to discuss the direction of charge transfer between the nanoparticle and the substrate. Despite the differences of the constructed band diagrams from the employed functionals, we consistently find the absence of charge transfer between the vacancy and the cluster, as well as a positive charging of the Au nanoparticle. The obtained results and their implication for the role of the vacancy in the catalytic system will be discussed.

O 29.7 Tue 12:00 H25

Template-Guided Programmable Janus Heteronanostructure Arrays for Efficient Plasmonic Photocatalysis — •Zhiqiang Zeng, Rui Xu, and Yong Lei — Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Abstract: Janus heteronanostructures (HNs) could facilitate synergistic coupling of diverse functions inherited by their comprised nanocomponents. Nowadays, synthesizing deterministically targeted Janus HNs remains a challenge. Here, a general yet scalable technique is utilized to fabricate an array of programmable Janus HNs based on binary-pore anodic aluminum oxide templates. The binary-pore anodic aluminum oxide templates provide high degrees of design freedom for both nanocomponents of the Janus HNs, including morphologies, compositions, dimensions, and interfacial junctions. Arrays of TiO2-Au and TiO2/Pt NPs-Au Janus HNs are prepared and demonstrated about 2.2 times photocurrent density and 4.6 times hydrogen evolution rate of that obtained from their TiO2 counterparts. The enhancement was mainly due to localized surface plasmon resonance induced direct hot electron injection and strong plasmon resonance energy transfer near the interfaces of TiO2 nanotubes and Au nanorods. This study may represent a promising step forward to pursue customized Janus HNs, leading to novel physicochemical effects and device applications.

O 29.8 Tue 12:15 H25

Structure and surface energies of nanoparticles from atomistic simulations — •David Holec[1], Franz Fischer[2], and Dieter Vollath[3] — [1]Department of Materials Science, Montanuniversität Leoben, Austria — [2]Franz-Josef-Strasse 18 — [3]NanoConsulting, Stutensee, Germany

Nanoparticles are fascinating objects not only from the point of view of diversity of their applications but also from the basic research perspective. In this contribution we review our recent activities directed towards revealing structure and surface energy of Au_{55} nanoparticle. It turns out that an amorphous structure possesses lower energy than a crystalline or well ordered structure. In this context, the two step process to increase the thermal stability should be mentioned. This process is a new, until now, never described phenomenon. Further on, we shown that surface energy changes dramatically as a function of the radius, in particular for a particle with small effective radius such as Au_{55}. This small change of radius is physically corresponding to the presence of an electronic cloud surrounding atomic radii. By calibrating our calculations to bulk fcc Au mass density we propose that the radius should be about increased by 0.13 nm as compared to convex hull of only ionic positions. Eventually, this correction of the surface energy radius makes is possible to put the contradictory trends from theory (surface energy increases with decreasing particle size) and experiment (surface energy decreases with decreasing particle size) onto a common ground, finally yielding only a slight-to-no particle size dependence.

O 29.9 Tue 12:30 H25

Soft Epitaxial Superlattices of PbS Nanocrystals — •Santanu Maiti[1,2], Alexander André[3], Sonam Maiti[2,3], Martin Hodas[2], Maciej Jankowski[4], Marcus Scheele[3], and Frank Schreiber[2] — [1]Institute of Complex Systems, Forschungszentrum Jülich, Germany — [2]Institute of Applied Physics, University of Tübingen, — [3]Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany — [4]ID10, European Synchrotron Radiation Facility, France

We prepare templates of atomically coherent, ordered superlattices of PbS NCs, coupled with copper tetraaminophthalocyanines (CuTAPc) molecules [1,2]. PbS NCs of different sizes/shapes are deposited on the surface of templates and the adlayer superlattices are further functionalized with CuTAPc [2]. Here, we investigate the structure of the templates as well as the adlayer NC assemblies by using grazing-incidence small angle x-ray scattering (GISAXS), grazing incidence x-ray diffraction (GIXD) and electron microscopy [3]. The deposited NCs self-assemble not only into ordered superstructures (sc, bcc), but also into a preferred atomic orientation with respect to the templates. Moreover, after functionalization, the bcc superlattices undergo a remarkable orientational change from [110]SL to [100]SL via lattice reconstruction. These results provide new insight into the coherent design of epitaxial nanostructures with desired crystallographic orientation [4,5]. [1] M. Scheele et al, PCCP 2015, 17, 97; [2] S. Maiti et al, JPCL 2018, 9, 739-744; [3] S. Maiti et al, JPCM 2017, 29, 095101; [4] S. M. Rupich et al, Nat Commun. 2014, 5, 5045; [5] M. X. Wang et al, ACS Nano 2017, 11, 180-185.

O 29.10 Tue 12:45 H25

Studying Copper Growth on Zinc Oxide Utilizing a Neural Network Potential — •Martín Leandro Paleico and Jörg Behler — Universität Göttingen, Theoretische Chemie, Tammannstr. 6, 37077 Göttingen, Germany

The catalyst used in the industrial synthesis of methanol is composed of large copper and zinc oxide nanoparticles. Studying this system requires a simulation method capable of handling thousands of atoms with ab initio accuracy, but with computational efficiency comparable to classical force fields. For this purpose, a Neural Network Potential (NNP) has been trained to reproduce the potential energy surface of the system, making use of DFT calculations as reference data.

The current work focuses on results for model ternary copper-zinc oxide system. Specifically, we investigate the growth of copper clusters and films on zinc oxide surfaces using both grid and grid-free basin hopping Monte Carlo simulations, entrenching of clusters at elevated temperatures and under an indentation force, and the behavior of copper and zinc oxide interfaces at high temperatures.

O 30: Surface Magnetism (joint session O/MA)

Time: Tuesday 10:30–13:00 Location: H37

O 30.1 Tue 10:30 H37

Unoccupied surface and interface states in thin film of Pd deposited on Fe/Ir(111) surface — •Mohammed Bouhassoune, Imara Lima Fernandes, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Pd layer deposited on Fe/Ir(111) substrate has been recently subject to intensive investigations since it hosts small swirling spin-textures named skyrmions that have potential interest in spintronic devices as magnetic bits for information technology. To manipulate and stabilize such non-collinear magetic objects it is of important demand to conduct a quantitaive study of their electronic structure. Here we aim to investigate the unoccupied states in Pd thin layers deposited on Fe/Ir(111) substrate using density functional theory. These unoccupied states are behind the large spin-mixing magnetoresisatnce (XMR) signature measured using non spin-polarized scanning tunnelling microscopy (STM) [1,2]. By analysing the electronic band structure we demonstrate the emergence of surface and interface states after deposition of Pd monolayers, which are very sensitive to the large spin-orbit coupling of Ir surface giving rise to the XMR signal.

This work is supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (ERC-consolidator Grant No. 681405 DYNASORE).

[1] D. M. Crum, M. Bouhassoune, J. Bouaziz, B. Schweflinghaus, S. Blügel, and S. Lounis, Nat. Commun. 6 8541 (2015)

[2] C. Hanneken et al, Nat, Nanotech. 10, 1039 (2015)

O 30.2 Tue 10:45 H37

Investigation of Fe/Pt (110) magnetic structure by first-principles methods — •Vasily Tseplyaev, Jens Bröder, Markus Hoffmann, Daniel Wortmann, Bernd Zimmermann, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

While skyrmions - localized and topologically protected vortex-like magnetic textures - are the main focus within the current research field of chiral magnets, we have discussed in a recent work [1] the possible emergence of interface stabilized *antiparticles*, so-called antiskyrmions, magnetic textures with a topological charge and one-dimensional winding number opposite to the one of skyrmions. For instance, antiskyrmions can appear in ultrathin magnetic films grown on heavy metal substrates with C_{2v} symmetry, if the electronic structure supports a Dzyaloshinskii spiralization tensor that fulfils additional conditions e.g. its determinant is smaller than zero. With the motivation to find interesting antiskyrmion systems we investigate magnetic systems with C_{2v} interface symmetry, e.g. Fe/Pt(110), using relativistic and non-collinear first-principles theory implemented in the FLEUR code (www.flapw.de).

[1] M. Hoffmann *et al.*, Nat. Commun. **8**, 308 (2017)

O 30.3 Tue 11:00 H37

Yu-Shiba-Rusinov states of Fe atoms on 2H-NbSe$_2$ — •Eva Liebhaber[1], Rojhat Baba[1], Jannik Steinborn[1], Gaël Reecht[1], Sebastian Rohlf[2], Kai Rossnagel[2], Benjamin W. Heinrich[1], Felix von Oppen[1,3], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Germany. — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany. — [3]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany.

A magnetic impurity adsorbed on a superconducting substrate induces Yu-Shiba-Rusinov (YSR) states. These are low-energy bound states inside the superconducting energy gap. The symmetry and extent of the YSR wave function depends on the adsorption site (i.e. crystal field), the nature of the orbital hosting the impurity's spin and the shape of the Fermi surface of the substrate.

We investigate single Fe atoms on 2H-NbSe$_2$. 2H-NbSe$_2$ belongs to the class of transition metal dichalcogenides (TMDCs) and is a layered van der Waals material with strong 2D character. In this material, superconductivity coexists with a charge density wave (CDW) at low temperatures. As the CDW is incommensurate with the lattice there are different local charge modulations present on the surface. Hence, adatoms sitting in identical hollow sites differ in their position relative to the CDW leading to variations in symmetry and energy of the YSR resonances.

O 30.4 Tue 11:15 H37

Epitaxial growth of the ultrathin EuS films on the InAs(001) and magnetic coupling between these films and organometallic phthalocyanine monolayers — •Carmen González Orellana, Maxim Ilin, and Celia Rogero — Centro de Física de Materiales, San Sebastián, Spain

EuS has recently attracted a lot of interest because of its ability of creating strong exchange fields when its placed in contact with non-ferromagnetic materials. For instance, at the interface between EuS and the topological insulator Bi_2Se_3, interfacial ferromagnetism was found to persist up to room temperature, despite the low Tc of bulk EuS (16.6 K). Furthermore, the formation of a new ferromagnetic ground state of the Dirac electrons in graphene was inferred on the basis of the electrical characterization of devices featuring a graphene/EuS interface.

I will present results of our work aimed to study the properties of the ultrathin EuS films and the interfaces between EuS and the organometallic pthalocyanines. We have optimized the epitaxial growth of EuS ultrathin films (< 1nm) on single crystal semiconducting InAs(001) substrates and characterized their structural and magnetic properties using LEED, STM, XPS, ex-situ magnetometry and in-situ XMCD techniques. Furthermore, we have grown monolayers of organometallic pthalocyanines (CuPC and MnPC) and performed XMCD measurements to probe the difference in the exchange coupling of the paramagnetic molecules with metallic (Ni, Co) and semiconducting (EuS) ferromagnets.

O 30.5 Tue 11:30 H37

Coordination-induced spin-state switching of a Ni complex on Ag(111) — •Manuel Gruber[1], Alexander Köbke[1], Florian Gutzeit[2], Rainer Herges[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, Germany

The spin state of a transition-metal complexes (TMC) can be controlled by changing its coordination state. For TMC on surfaces, this was so far realized by adding/removing gaseous molecules [1] or by transferring a ligand (e.g. Cl) with the tip of a scanning tunneling microscope (STM) [2]. Alternatively, a switching unit within the TMCs itself may be employed to change the coordination state of the complex [3], but so far the interaction with the substrate was detrimental for the molecular structure and switching properties [4].

In the present study, we have designed and investigated robust Ni complexes, which can intrinsically switch their coordination state. Combining low-temperature scanning tunneling microscopy, near-edge x-ray absorption spectroscopy along with density functional theory calculations, we evidence the switching of these complexes on Ag(111) between the S=0 and S=1 spin states.

This work was supported by the DFG through SFB 677 and the European Union's Horizon 2020 programme (No. 766726). [1] Gopakumar et al., J. Am. Chem. Soc. **134**, 11844 (2012) [2] Wäckerlin et al., Adv. Mater. **25**, 2404 (2013) [3] Venkataramani et al., Science **331**, 445 (2011) [4] Matino et al., Chem. Commun. **46**, 6780 (2010)

O 30.6 Tue 11:45 H37

Magnetic order in Nd(0001): a new type of spin glass? — •Umut Kamber, Andreas Eich, Nadine Hauptmann, Daniel Wegner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

Lanthanide metals can exhibit complex magnetic structures, e.g. helical/conical spin spirals or linear spin waves. Neodymium (Nd) shows the most complicated behavior exhibiting several magnetic phase transitions below TN = 19.9 K, resulting in multi-q order according to interpretations based on magnetic neutron or X-ray diffraction experiments [1]. However, as these techniques lack spatial resolution, the variations in magnetic properties of Nd at the atomic length scale are unexplored. The local surface electronic structure of Nd(0001) has been studied only using spin-integrated STS [2,3]. Here, we present ultra-low temperature SP-STM measurements of bulk-like Nd(0001) films grown on W(110). We observe multi-q magnetic behavior on the surface as evidenced by strong short-range order, but without the existence of long-range order. Magnetic field and temperature-dependent measurements reveal high sensitivity of the spectral weight of q-states to applied fields, without any clear unique ground state, as well as evidence of aging behavior in the magnetic state. We discuss our findings in the context of unconventional spin-glass behavior. [1] R. M. Moon & R. M. Nicklow, J. Magn. Magn. Mater. 100, 139 (1991). [2] D. Wegner et al., Phys. Rev. B 73, 165415 (2006). [3] D. Wegner et al., Jpn. J. Appl. Phys. 45, 1941 (2006).

O 30.7 Tue 12:00 H37

On the magnetic coupling characteristics of endohedral fullerenes on Au(111) and Cu(111) by scanning tunneling microscopy (STM)/ spectroscopy (STS) and X-ray magnetic circular dichroism (XMCD) — •Emmanouil Koutsouflakis, Lukas Spree, Georgios Velkos, Yaofeng Wang, Sebastian Schimmel, Danny Baumann, Bernd Büchner, Christian Hess, and Alexey Popov — IFW-Dresden, 01069 Dresden, Germany

Single-Molecule Magnets (SMMs) are molecular materials whose molecules may exhibit magnetic properties such as magnetization under zero-field conditions, large relaxation times and high blocking temperatures. Towards molecular electronics and the subsequent controlled manipulation of single spins in SMMs, the obstacle of the insufficient chemical stability of many SMM architectures has to be overcome, in order to facilitate both their organization on substrates and the preservation of their properties.

We report on the alternatives of Trimetallic Nitrides (TNTs) and Dimetallic Fullerenes. TNTs are of the type $A_{3-n}B_nN@C_{80}$ (n=0-3; A, B rare earth metals or transition metals) where a carbon cage encapsulates a triangular cluster of three rare earth/ transition metal atoms and a nitrogen at its center. In dimetallic fullerenes the cluster is consisted of two lanthanide ions forming a covalent bond by an unpaired electron. In situ sub-monolayers on Au(111) and Cu(111) substrate have been developed under UHV conditions and STM/ STS and XMCD techniques have been applied to investigate the disruptive effects that arise on depositing SMMs onto reactive metal surfaces.

O 30.8 Tue 12:15 H37

Effect of the Li doping on the Curie temperature of the GdAu2 surface alloy — •M. Ilyn[1,2], M. Gobbi[1,2], C. Rogero[1,2], P. Gargiani[3], M. Valbuena[4], C. Moreno[4], A. Mugarza[4,5], and F. Schiller[1,2] — [1]Materials Physics Center CSIC-UPV-EHU — [2]Donostia International Physics Center — [3]ALBA Synchrotron — [4]Catalan Institute of Nanoscience and Nanotechnology (ICN2) — [5]ICREA Institució Catalana de Recerca i Estudis Avançats

Magnetic surface alloys REAu2 (where RE stands for the rare-earth elements) are the two-dimensional counterparts of the 3-D intermetallic compounds. They were found to be a model system to study the magnetic phenomena in 2-D metallic materials. Indeed, grown on the single-crystal substrates they have atomically-flat surface and a long-range crystallographic order, allowing for use of all standard surface science techniques. On the other hand, magnetic properties of this system can be tuned via choosing the RE element or a noble metal of the substrate.

In this talk I will present results that show the effect of Li doping on the magnetic properties of GdAu2 surface alloy. Previously we have seen that GdAu2 retains its magnetic properties when it is interfaced with organic layers and sustains a thermally activated dehalogenation reaction, but its Curie temperature (Tc) decreases. New XMCD measurements demonstrate a strong (by 60%) growth of the Tc in GdAu2 due to the evaporation of the submonolayer amount of Li. These data together with results of the XPS and ARPES measurements will be used to discuss the mechanism of the observed phenomena.

O 30.9 Tue 12:30 H37

Disentangling spin-dependent scattering processes in thin Tb and Gd films — Gesa Siemann, •Wibke Bronsch, Beatrice Andres, and Martin Weinelt — Freie Universität Berlin, Deutschland

Studying the magnetic phase transition in thin Gd and Tb films by spin-resolved photoemission spectroscopy, we evaluated the linewidth of the (0001) surface state as a function of temperature in accordance with Ref.[1]. We observe different linewidths for the majority and minority spin components of the spin-mixed occupied surface state indicating differing scattering channels and concomitant spin-dependent lifetimes. A linear increase of the linewidth with temperature for $T > T_{\mathrm{Debye}}$ allows us to evaluate the electron-phonon scattering rate. We find a larger slope for the majority-spin channel compatible with the higher density of bulk states for majority spin electrons at $T < T_{\mathrm{Curie}}$. Furthermore, we observed a greater Lorentz width for the minority-spin component, which is attributed to electron-magnon scattering. The contributions of electron-phonon and electron-magnon scattering to the linewidth of the surface state are comparable for Gd and Tb.

[1] Fedorov *et al.*, Phys. Rev. B **65**, 212409 (2002)

O 30.10 Tue 12:45 H37

Disentangling the double-exchange and superexchange interactions in quantum anomalous Hall insulators — •Thiago R. F. Peixoto[1], Hendrik Bentmann[1], Abdul-Vakhab Tcakaev[2], Philipp Rüssmann[3], Raphael Crespo Vidal[1], Sonja Schatz[1], Fabian Stier[2], Volodymyr Zabolotnyy[2], Martin Winnerlein[4], Steffen Schreyeck[4], Charles Gould[4], Karl Brunner[4], Stefan Blügel[3], Laurens W. Molenkamp[4], Vladimir Hinkov[2], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg — [2]Experimentelle Physik IV, Universität Würzburg — [3]Peter Grünberg Institut (PGI-1), Forschungszentrum Jülich — [4]Experimentelle Physik III, Universität Würzburg

We report on the electronic origin of the magnetic properties of the quantum Hall insulators (V,Cr):(Bi,Sb)$_2$Te$_3$. By combining x-ray magnetic circular dichroism (XMCD), resonant photoemission spectroscopy (resPES) and density functional theory (DFT), we trace element-specific fingerprints in the valence band and magnetic coupling mechanisms. Our results show that while the low spectral weight of Cr $3d$ states at the Fermi level (E_F) support the presence of ferromagnetic superexchange interactions, an additional double-exchange interaction is intimately related to a highly localised V $3d$ impurity band at E_F. Furthermore, we show that a Bi-rich host increases the covalency of the transition metal ions, thereby mitigating Hund's rule stabilisation. The competition between charge-transfer and *pd*-exchange ultimately determines the magnetic ground-state in these systems [1].

[1] Larson and Lambrecht, Phys. Rev. B **78**, 195207 (2008).

O 31: Plasmonics & Nanooptics II: SHG and Dielectric Properties (joint session O/CPP)

Time: Tuesday 14:00–16:30 Location: H8

O 31.1 Tue 14:00 H8

Sum-Frequency Generation Enhanced by Localized Surface Phonon Polaritons — •Riko Kiessling[1], Yujin Tong[1], Alexander J. Giles[2], Joshua D. Caldwell[2,3], Martin Wolf[1], and Alexander Paarmann[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]U.S. Naval Research Laboratory, Washington, D.C., USA — [3]Vanderbilt University, Nashville, USA

Nanophotonic devices open the way to tailor light-matter interaction on the nano-scale by specifically designed structures of solid-state material. This is advantageous for, e.g., the sub-diffractional localization of light, which fosters amplification of nonlinear optical frequency conversion processes by enhancement of local electric fields.

Here, we employ localized surface phonon polariton modes in nanostructured polar dielectric media [1] to resonantly increase the nonlinear response. In contrast to surface plasmons, the optical phonon-based approach exhibits significantly lower optical losses. By means of IR-VIS sum-frequency generation spectroscopy [2], a strong modulation of the local electromagnetic fields, and thus, amplified upconversion radiation, is observed. Intensity and spectral position of the nonlinear emission can be manipulated by the nanostructure design. In this way, sub-wavelength sized architectures prove to be an efficient method for the control of localized fields associated with three-dimensionally confined optical modes in the mid-infrared spectral region.

[1] Razdolski et al., Nano Lett. 16, 6954 (2016)

[2] Kiessling et al., Phys. Rev. Accel. Beams 21, 080702 (2018)

O 31.2 Tue 14:15 H8

Nonlinear Response of Grating-Coupled Surface Phonon Polaritons — Marcel Kohlmann, Nikolai Christian Passler, Martin Wolf, and •Alexander Paarmann — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Surface Phonon Polaritons (SPhPs) have recently attracted much attention in infrared nanophotonics, due to their low losses compared to plasmon polaritons. Specifically for nonlinear optics, SPhPs result in tremendous enhancement of local optical fields [1,2]. Here, we study the nonlinear response of grating-coupled SPhPs [3] in by means of second-harmonic generation (SHG), in sub-wavelength SiC grating geometries. Non-specular emission of SHG is observed for resonant SPhP excitation, demonstrating the peculiarities of nonlinear scattering for grating-coupled nonlinear nanophotonics [4].

[1] Razdolski et al., Nano Letters 16, 6954 (2016).

[2] Passler et al., ACS Photonics 4, 1048 (2017).

[3] Greffet et al., Nature 416, 61 (2002).

[4] Quail and Simon, J. Opt. Soc. Am. B 5, 325 (1988).

O 31.3 Tue 14:30 H8

Wavelength-dependent Third Harmonic Generation in Metallic Thin Films — •Vincent Drechsler, Joachim Krauth, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Harmonic generation in plasmonic systems has gained significant interest in the last years. While the plasmonic near-field enhancement has been studied in great detail, little attention was paid to the origin of the nonlinear signals which in fact lie in the microscopic nonlinearity of the involved plasmonic metals. In order to predict wavelength-dependent nonlinear processes it is therefore crucial to understand these microscopic nonlinearities. Utilizing an optical parametric oscillator as a tunable broadband light source, we study wavelength-dependent third harmonic generation from metallic thin films made of Gold, Copper, and Magnesium. We find that the linear properties of the metallic films, that is their absorption, strongly influence the third harmonic generation efficiency. Optical transitions between the different bands lead to a resonant enhancement of the third order susceptibilities. Utilizing hydrogen to switch metallic magnesium to dielectric magnesium hydride we can tune the nonlinearity of thin films and observe the metallic-dielectric phase transition in the linear and nonlinear regime. We find complex relations between the linear transmittance and the radiated third harmonic, which provide new insights into the phase transition.

O 31.4 Tue 14:45 H8

Plasmonic analogue of Electromagnetically Induced Absorption Boosts Third Harmonic Generation — •Joachim Krauth, Mario Hentschel, Bernd Metzger, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

In three-dimensional nanostructures, the appropriate choice of geometry and materials allows for tailoring the linear optical properties in a vast range. In the so-called plasmonic dolmen structure the coupling between a bright and a dark state can be manipulated to realize the plasmonic analogue of electromagnetically induced absorption (EIA), resulting in an enhanced absorbance of the coupled system. In analogy to solid state nonlinear optics, in which the linear absorption spectra largely determine the nonlinear interaction, plasmonic EIA is therefore expected to boost nonlinear conversion efficiencies. We are reporting third harmonic generation spectroscopy results on a plasmonic EIA system. The radiated third harmonic signals can be understood when taking the intricate phase relation and coupling strength dependence of EIA into account. An appropriately modified anharmonic oscillator model based on the linear absorption spectra can describe the nonlinear response of our three-dimensional plasmonic structure. The design freedom associated with three-dimensional nanostructuring can provide further insight into the nonlinear response of complex plasmonic systems.

O 31.5 Tue 15:00 H8

Symmetry-forbidden second-harmonic generation in a fully centro-symmetric plasmonic nanocircuit — •Julian Obermeier[1], Tzu-Yu Chen[2], Thorsten Schumacher[1], Fan-Cheng Lin[2], Jer-Shing Huang[3,4,5], Chen-Bin Huang[2,5], and Markus Lippitz[1] — [1]University of Bayreuth, Germany — [2]National Tsing Hua University, Taiwan — [3]Leibniz Institute of Photonic Technology, Germany — [4]National Chiao Tung University, Taiwan — [5]Research Center for Applied Sciences, Taiwan

Nonlinear optical frequency conversion on the nanoscale remains a challenge, but may pave the path towards multi-functional optical circuits. Surface plasmon fields are highly spatially confined near the metal/dielectric interface and exhibit giant field enhancement. These two attributes are invaluable for nonlinear optics with plasmons. However, second-harmonic generation in bulk is forbidden in centrosymmetric materials such as typical noble metals. Past efforts concentrated on the broken symmetry at the surface in combination with an asymmetric shape of the particle. We introduce a new way of breaking the symmetry by a propagating mode of a plasmonic waveguide, a two-wire transmission-line. We demonstrate that an optical mode of correct symmetry is sufficient to allow SHG even in centro-symmetric structures made of centro-symmetric material. This is a new degree of freedom for on-chip nonlinear signal processing in nanophotonics.

O 31.6 Tue 15:15 H8

Resonant Field Enhancement of Epsilon Near Zero Berreman Modes in an Ultrathin AlN Film — •Nikolai Christian Passler[1], Ilya Razdolski[1], Joshua D. Caldwell[2], Martin Wolf[1], and Alexander Paarmann[1] — [1]Fritz-Haber-Institute of the MPG, Berlin, Germany — [2]Vanderbilt University, Nashville, USA

In nanophotonics, the strongly enhanced local optical fields of polaritonic modes are the driving force of nonlinear optical phenomena. In sub-wavelength thin polar dielectric films, a polaritonic Berreman mode arises at the longitudinal optical phonon frequency where the dielectric permittivity crosses zero [1]. Complementary to this radiative epsilon near zero (ENZ) mode, also an evanescent ENZ polariton is supported at large in-plane momenta [2], exhibiting similar properties. At resonance, the Berreman mode features an immense field enhancement, enabling to boost the efficiency of nonlinear nanophotonic applications like all-optical ultrafast switching.

Employing a mid-infrared free-electron laser, we investigate the second harmonic generation (SHG) of an ultrathin AlN layer on top of bulk SiC. The employed SHG spectroscopy [3] serves as a direct experimental probe of the tremendous field enhancement of the high-quality, strongly confined ENZ Berreman mode. With these properties, the AlN thin-film Berreman mode offers an appealing platform for the development of novel infrared nanophotonic devices.

[1] Vassant et al., Optics Express 20, 23971 (2012)
[2] Passler et al., Nano Letters 18, 4285 (2018)
[3] Paarmann et al., Applied Physics Letters 107, 081101 (2015)

O 31.7 Tue 15:30 H8

Enhanced second harmonic emission from zinc oxide nanoparticles infiltrated into the pores of gold nanosponges — •Jue-Min Yi[1], Dong Wang[2], Felix Schwarz[3], Jinhui Zhong[1], Abbas Chimeh[1], Anke Korte[1], Peter Schaaf[2], Erich Runge[3], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, 26129 Oldenburg — [2]TU Ilmenau,98693 Ilmenau. — [3]TU Ilmenau, 98693 Ilmenau

We introduce zinc-oxide (ZnO)-functionalized porous gold (Au) nanoparticles which exhibit strong second harmonic (SH) generation around 400 nm by coupling surface plasmons (SPs) to ZnO excitons. The hybrid nanosystem consists of a thin layer (˜10 nm) of ZnO incorporated into individual porous Au nanoparticles percolated with a three-dimensional (3D) network of 10-nm sized ligaments acting as nanoantennas and nanocavities.We have utilized a broadband and few-cycle ultrafast laser to generate coherent nonlinear emission from individual bare nanosponges and from ZnO-functionalized sponges. The third harmonic (TH) emission spectrum of Au/ZnO hybrid particles reveals a distinct red shift with respect to pure Au sponges. In contrast, a substantial broadening of the SH spectra and a distinct blue-shift is seen in the ZnO-functionalized nanosponges. It is demonstrated that SH emission around 400 nm, close to the ZnO band gap, is 15 times stronger with respect to bare Au nanosponges. Such enhanced SHG emission is attributed to plasmon-enhanced two-photon excitation of ZnO excitons.

O 31.8 Tue 15:45 H8

Revealing Plasmon-Exciton Coupling for SHG Enhancement by Interferometric Frequency Resolved Autocorrelation — •Jinhui Zhong[1], Juemin Yi[1], Dong Wang[2], Anke Korte[1], Abbas Chimeh[1], Peter Schaaf[2], and Christoph Lienau[1] — [1]Institute of Physics, Carl von Ossietzky University Oldenburg, 26129 Oldenburg, Germany — [2]Institut für Mikro- und Nanotechnologien MacroNano and Institut für Werkstofftechnik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Plasmon-enhanced excitonic nonlinear emission from semiconductors is interesting because the coupling of plasmon and exciton may boost the nonlinear generation efficiency. Nevertheless, to date, a detailed characterization of the electron dynamics of metal(plasmon)-semiconductor(exciton) composites is lacking. Herein, we present interferometric frequency-resolved autocorrelation (IFRAC) measurements on individual porous gold nanoparticles (nanosponges) incorporated with ZnO that allows us to track spectrally and temporally the response of the generated second-harmonic fields. We propose a method to distinguish homogeneous and inhomogeneous spectral broadening of plasmon resonances by Fourier-transform of the IFRAC traces to get two-dimensional (2D) IFRAC spectra. More importantly, we observed enhanced excitonic SHG emission at 390 nm from ZnO by coupling to localized plasmons of gold nanosponges. Pronounced features of coherent plasmon coupling are observed, proving that localized plasmons enhance the nonlinear ZnO excitonic emission, as revealed from the fundamental (FM) sidebands of the 2D spectra.

O 31.9 Tue 16:00 H8

Low-temperature infrared dielectric function of hyperbolic α-quartz — •Christopher J. Winta, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Natural hyperbolic materials, where the principal components of the dielectric tensor have opposite signs, like hexagonal boron nitride [1], have recently attracted much attention due to their unique characteristics for polaritonic nanophotonics [2]. Here, we show that also the common uniaxial crystal α-quartz exhibits multiple hyperbolic bands in the far-infrared (far-IR), which support low-loss hyperbolic modes at low temperatures.

We determine the IR dielectric properties of α-quartz in the temperature range from 1.5 K to 200 K. Far-IR reflectivity spectra of a single crystal y-cut were acquired in 8 distinct configurations. Fitting a multi-oscillator model globally to these data allows for extraction of frequencies as well as damping rates of the in-plane and out-of-plane, the longitudinal and transverse IR-active optic phonon modes, and hence the temperature-dependent ordinary and extraordinary dielectric functions, $\varepsilon_\perp(\omega)$ and $\varepsilon_\parallel(\omega)$, respectively.

The results are consistent with previous high temperature studies [3] and indicate remarkably high quality factors, Q, for polaritons at low temperatures in α-quartz's hyperbolic spectral region.

[1] Caldwell et al., *Nature Communications* **2014**, *5*.
[2] Liu, Lee, Xiong, Sun, Zhang, *Science* **2007**, *315*, 1686–1686.
[3] Gervais and Piriou, *Phys. Rev. B* **1975**, *11*, 3944–3950.

O 31.10 Tue 16:15 H8

Tunable Low Loss 1D Surface Plasmons in InAs Nanowires — •Yixi Zhou[1], Jianing Chen[1], and Thomas Taubner[2] — [1]Institute of Physics, CAS — [2]Institute of Physics (IA), RWTH Aachen

Due to the ability to manipulate photons at the nanoscale, plasmonics has become one of the most important branches in nanophotonics [1]. The prerequisites for the technological application of plasmons include high confining ability ($\lambda_0/\lambda_\mathrm{p}$), low damping, and easy tunability. However, plasmons in typical plasmonic materials, i.e. noble metals, cannot satisfy these three requirements simultaneously, therefore limiting their overall applicability [2].

Here, indium arsenide (InAs) nanowires are identified as a material that satisfies all three prerequisites, providing a platform for modern nanophotonics. The dispersion relation of InAs plasmons is determined using the nanoinfrared imaging technique, and show that their associated wavelengths and damping ratios can be tuned by altering the nanowire diameter and dielectric environment. The launched plasmons simultaneously exhibit high confinement factor ($\lambda_0/\lambda_\mathrm{p} = 34$) and low damping rate ($\gamma^{-1} = 25$) [3]. The observation of InAs plasmons could enable novel plasmonic circuits for future subwavelength applications.

[1] J. A. Schuller et al., Nat. Mater. 9, 193 (2010).
[2] D. K. Gramotnev et al., Nat. Photonics. 4, 83 (2010).
[3] Y. Zhou et al., Adv. Mater. 30, 1802551 (2018).

O 32: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge IV (joint session O/CPP/DS/TT)

Time: Tuesday 14:00–16:45 Location: H9

Topical Talk O 32.1 Tue 14:00 H9

The Data Revolution in Materials Science, Through the Lens of the Materials Project — •Kristin Persson — University of California, Berkeley, USA

Advanced materials are essential to economic and societal development, with applications in multiple industries, from clean energy, to national security, and human welfare. Historically, novel materials exploration has been slow and expensive, taking on average 18 years from concept to commercialization. Due to the tremendous improvements in computational resources, coupled with software development during the last decades, real materials properties can now be calculated from quantum mechanics much faster than they can be measured. A new era of computational materials prediction and design has been born. A result of this paradigm change are databases like the Materials Project which is harnessing the power of supercomputing together with state of the art quantum mechanical theory to compute the properties of all known inorganic materials and beyond, design novel materials and offer the data for free to the community together with online analysis and design algorithms. We leverage the rich data from the Materials Project for machine learning; accelerating materials design, characterization and finally synthesis of materials. This talk will survey this rapidly evolving and exciting paradigm in science, showcasing the possibilities and iteration between ideas, computations, insight and new materials development.

O 32.2 Tue 14:30 H9

High-throughput simulations of complex band structure — •Emanuele Bosoni and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2

The Complex Band Structure (CBS) generalizes the conventional band structure of a material by considering wave-vectors with complex components. The CBS extends the description of the allowed states of a material beyond the bulk propagating states, including in the picture the evanescent wave-functions that grow or decay from one unit cell to the next. Even though these latter states are forbidden by translational symmetry, they become important when this is broken via, for example, an interface. In the past, many studies made use of CBS calculations in order to confirm or motivate experimental findings, but only recently we see some efforts to give an unified prospective to the study of this quantity [1]. Moreover, the growth in recent years of high-performance computational resources available at relatively low cost opens the possibility to make a systematic, high-throughput, study of the CBS within the Density Functional Theory (DFT) framework.

In this contribution we will present our implementation of the Transfer Matrix Method [1] for the calculation of the CBS within the DFT code Siesta [2] and we will explain challenges and benefits of the high-throughput approach. We will present a proof of concept example in which we calculated the CBS for a set of materials and we will conclude explaining the relevance of our project in the field of spintronics.

[1] Reuter M. G., J. Phys.: Condens. Matt. 29, 053001 (2017)

[2] J. M. Soler et al., J. Phys.: Condens. Matt. 14, 2745 (2002)

O 32.3 Tue 14:45 H9

Computational Screening of 2D Materials for Solar Cells Application — •Anders Christian Riis-Jensen and Kristian Sommer Thygesen — Institute for Physics, Technical University of Denmark

Two-dimensional (2D) materials have attracted great attention in recent years, not least due to their extremely strong coupling to light and pronounced excitonic effects. This makes 2D materials an ideal playground for studying light-matter interaction in nano-scale materials for applications within e.g. solar cells and photo-detectors. In this work, we present a large-scale computational study of a wide variety of 2D materials with the aim of identifying novel candidates with strong light-matter interaction. Specifically, we calculate the absorption spectrum of almost 2000 materials at the level of the Random Phase Approximation (RPA) and/or by solving the Bethe-Salpeter Equation (BSE). This enables us of calculating the Power Conversion Efficieny (PCE) for all these materials fully ab-initio. Based on this we identify specific 2D semiconductors for both single- and tandem solar cells. The best candidates present power densities (PCE per unit mass) of several orders of magnitude larger than both Si and GaAs. Lastly, we also show a detailed analysis of a few 2D materials, in which we find exciton states with exceptionally strong coupling to light and large exciton binding energies.

O 32.4 Tue 15:00 H9

First-principles Modelling of Solid-Solid Interfaces in all Solid-State Batteries — •Bora Karasulu[1], James P. Darby[1], Clare P. Grey[2], and Andrew J. Morris[3] — [1]Dept. of Physics, Univ. of Cambridge, UK — [2]Dept. of Chemistry, Univ. of Cambridge, UK — [3]School of Metallurgy and Materials, Univ. of Birmingham, UK

All solid-state batteries (ASSBs) can potentially mitigate the safety issues known for conventional Li-ion batteries, and provide enhanced energy densities, by replacing the organic electrolyte solutions with solid inorganic equivalents. Mechanical and (electro)chemical incompatibilities between the ASSB solid components, however, lead to high resistances, curtailing the Li-ion transport at their interfaces. In this talk, we introduce a high-throughput ab initio modelling approach towards the rational design of electrolyte/electrode interfaces in ASSBs. First, we obtain phase diagrams of sulfide-based electrolytes with diverse compositions, phases, vacancies and doping using the Ab Initio Random Structure Searching (AIRSS) method. Next, the stable and low-lying metastable phases are screened for their ionic conductivity using ab initio molecular dynamics simulations. Finally, diverse surfaces of the selected electrolyte phases are interfaced with the surfaces of electrodes or other interfacial (e.g. solid electrolyte interphase, SEI) layers to determine the stable combinations using an automated procedure (INTERFACER). The devised approach will be demonstrated in action for a collection of interfaces, e.g. Li-P-S electrolytes with LiCo2, Li-metal electrodes and alike.

O 32.5 Tue 15:15 H9

New Insights into Amorphous Materials and their Surfaces by Combining Machine Learning and DFT — •Volker Deringer — University of Cambridge, Cambridge, UK

Understanding links between atomic structure, chemical reactivity, and physical properties in amorphous solids is a long-standing challenge. DFT-based atomistic simulations have played important roles in this, but come at high computational cost. Novel interatomic potentials based on machine learning (ML) achieve close-to DFT accuracy, but require only a small fraction of the cost. In this talk, I will argue that such ML-based potentials are particularly useful for studying amorphous solids.

First, I will describe a Gaussian Approximation Potential (GAP) for amorphous carbon, which we recently used to simulate the deposition of tetrahedral amorphous carbon (*ta*-C) films, one atom at a time. These simulations reproduced the experimentally observed count of sp^3 atoms and gave new insight into the microscopic growth mechanism. I will then discuss how ML-based potentials can be combined with density-functional methods to yield new insights into surface functionalization (specifically, hydrogenation and oxidation) of *ta*-C. Finally, I will present recent work on amorphous silicon, another prototypical non-crystalline material that ML-driven simulations can describe with high accuracy. Looking ahead, these studies suggest that ML-based potentials may become more widespread tools for the realistic modelling and understanding of the amorphous state.

O 32.6 Tue 15:30 H9

Harvesting from unbiased sampling of open systems: phase diagrams and property maps of surfaces and clusters in reactive atmosphere — •Yuanyuan Zhou, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Numerous processes that occur at surfaces of materials play a critical role in the manufacture and performance of functional materials, e.g., electronic, magnetic, and optical devices, sensors, catalysts, and coatings. A prerequisite for analyzing and understanding the electronic properties and the function of surfaces is detailed knowledge of the atomic structure, i.e., the surface composition and geometry under realistic condition. We introduce a Replica-Exchange (RE) Grand-Canonical (GC) Monte-Carlo algorithm. By means of the coupled sampling at several chemical potentials (i.e., partial pressures) of a reactive gas atmosphere and temperatures, the REGC scheme enables the unbiased calculation of (p, T) phase diagrams of surfaces, nanoparticles, or clusters in contact with reactive atmosphere, where all anharmonic contributions are included. Moreover, the multi-canonical sampling yields the temperature-pressure dependence (map) of all equilibrium observables that can be measured within the given model Hamiltonian. For instance, structural parameters such as the radial distribution function, or the fundamental electronic gap. This allows for rational design, where *operando* condition are taking fully into account. We demonstrate the approach for model Lennard-Jones surfaces as well as Si clusters and surfaces in a hydrogen atmosphere.

O 32.7 Tue 15:45 H9

Crystal structure prediction for high capacity battery materials — •Angela F Harper[1] and Andrew J Morris[2] — [1]Department of Physics, University of Cambridge, JJ Thomson Ave, Cambridge CB3 0HE, UK — [2]School of Metallurgy and Materials, University of Birmingham, Edgbaston, Birmingham, UK

The future of large-scale energy storage relies heavily on the ability of Li-ion batteries to have high capacity and long-term stability. At present, graphite anodes limit the overall capacity of Li-ion batteries to a theoretical maximum of 372 mAh/g, and thus there is a need for higher capacity anodes such as phosphorus. We have studied lithiation in phosphorus using a combination of *ab initio* random structure searching (AIRSS) and density-functional theory calculations. In the Li-P system we found a novel phase of $P2_12_12_1$ Li_4P_3, which showed stable 0K phonon modes [1]. We further showed, using defect AIRSS searches, that doping the known Li-P phases with aluminium improved their electronic density of states at the Fermi level, and could improve conductivity in phosphorus anodes. To improve the cyclability of these phosphorus anodes, which break down after several cycles due to volume expansion of over 200%, in this talk we will investigate the phase diagrams and voltage profiles of several ternary compounds of Li-P-M where M is a metallic element which maintains the conductivity of aluminium doping and adds stability to the anode.

[1] Mayo, M. et al. Chem. Mater. 2016, 28, 2011*2021

O 32.8 Tue 16:00 H9

Constructing Accurate Machine Learning Force Fields for Flexible Molecules — •Valentin Vassilev-Galindo, Igor Poltavsky, and Alexandre Tkatchenko — Physics and Material Science Research Unit, University of Luxembourg, Luxembourg

State-of-the-art machine learning (ML) models can reproduce potential energy surfaces (PES) for molecules containing up to a few tens of atoms with the accuracy comparable to the most exact ab initio methods. This provides a unique tool for computing different thermodynamic properties that would require millions of CPU years otherwise. For instance, a recently developed sGDML[1,2] model predicts forces and energy with CCSD(T) accuracy using just a few hundreds of configurations for training. However, up to now ML has been mainly applied to rather rigid molecules. In this regard, our objective is to test ML for flexible molecules and out-of-equilibrium configurations along transition paths. For this, we select molecules (e.g. azobenzene, stilbene) with relatively complex transition paths, which result from an interplay between long- and short-range interactions. Then, different paths connecting PES minima are tested using sGDML. This allows us to define optimal descriptors and the most appropriate strategies for choosing the training sets, which is crucial for ML models relying on a limited number of training points. Our results open an avenue for efficiently calculating transport pathways, transition rates and other out-of-equilibrium properties with previously unattended accuracy.

[1] Chmiela, S. et al., Sci. Adv. 3, e1603015 (2017).

[2] Chmiela, S. et al., Nat. Commun. 9, 3887 (2018).

O 32.9 Tue 16:15 H9

Calculating critical temperatures for magnetic order in two-dimensional materials — •Daniele Torelli — CAMD, Department of Physics, Technical University of Denmark, 2820 Kgs. Lyngby, Denmark

Recent observation of ferromagnetic out-of-plane order in two-dimensional (2D) CrI_3 highlights the importance of a microscopic understanding of magnetic anisotropy (MA) in ground state magnetic systems. Single-ion anisotropy and anisotropic exchange coupling comprise crucial ingredients to escape the Mermin-Wagner theorem which implies that rotational symmetry cannot be spontaneously broken at any finite temperature in 2D and thus prevents magnetic order.

In the present work we investigate the variation of critical temperature in Heisenberg model systems using classical Metropolis Monte Carlo simulations. A fit for square, hexagonal and honeycomb lattices leads to a simple expression for the critical temperatures as a function of MA and exchange coupling constants.

Based on a new developed computational 2D materials database, we predict 2D structures with high critical temperatures and high thermodynamic and dynamic stability for future experimental investigations. As testing system, relevant Heisenberg exchange couplings and MA energies in mono-layer CrI_3 are obtained from first principle calculations and energy mapping analysis, yielding to an estimation of Curie temperature in good agreement with experimental results.

O 32.10 Tue 16:30 H9

Amino-acids on metallic surfaces: searching conformational space — •Dmitrii Maksimov, Carsten Baldauf, and Mariana Rossi — Fritz-Haber-Institut der Max-Planck- Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Organic-inorganic interfaces are challenging for computational modeling, in particular regarding the prediction of stable configurations at the interface, which determine the electronic properties of the system as a whole. The amino acid arginine is a flexible molecule in the gas phase and experiments show its self-assembly into dimers, rings, and chains on Ag(111) and Au(111) surfaces. For two protonation states (neutral Arg and charged $ArgH^+$), we perform systematic structure searches by placing known gas-phase minima in different orientations on top of the surfaces, followed by full relaxation within long-range dispersion corrected density-functional theory (DFT). In the analysis, we aim at understanding the alterations of the conformational space from the gas phase to surface adsorption by means of a dimensionality-reduced representation based on a combination of the Smooth Overlap of Atomic Positions (SOAP) and the Sketchmap techniques [1]. The favorable interaction with the metallic surface reduces the number of accessible conformations for neutral Arg. For the adsorption of charged $ArgH^+$, the number of local minima increases due to surface-dependent partial charge screening. [1] S. De et al., *J. Cheminform.*, **9**:6 (2017)

O 33: Solid-Liquid Interfaces III

Time: Tuesday 14:00–16:15 Location: H10

O 33.1 Tue 14:00 H10

Interaction of ethylene carbonate and lithium on thin cobalt oxide films - A model of the electrode|electrolyte interphase in Li-ion batteries — •Jihyun Kim[1], Florian Buchner[1], and R. Jürgen Behm[1,2] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89081 Ulm, Germany

In this model study, we aim to get a molecular scale understanding of the initial stages of the formation of the electrolyte interphase (SEI) at the electrode|electrolyte interface, which plays a critical role in the performance of Li ion batteries (LIBs). Here, we report on the interaction of ethylene carbonate (EC, main electrolyte component in LIBs) with a thin film of CoO(111) grown on Ru(0001), which was investigated by X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectroscopy (FTIRS) under UHV conditions. EC adsorbs molecularly intact on CoO(111) at 80 K and is stable below 200 K, while above 240 K EC decomposition is initiated. To mimic the electrolyte, 0.5 - 2 ML of Li was stepwise post-deposited on an EC adlayer at 80 K, which leads to EC decomposition most likely into Li-containing -C=O, -C-O-C-, -C-H species as well as Li_2O_2 or LiOH. For CoO anodes in LIBs, lithiation leads to a conversion reaction of CoO into Co^0 as well as Li_2O. However, for Li doses on EC adlayer at 80 K, we hardly observe such a reaction, indicating that Li directly interacts with EC. Only for Li doses on pristine CoO at 300 K, Co^0 forms in the near surface regime. The results demonstrate the initial stage of the chemical SEI formation as well as the conversion of CoO.

O 33.2 Tue 14:15 H10

The ionic liquid|cobalt oxide interface and interaction with lithium - A model study for the solid|electrolyte interphase in Li-ion batteries — •Florian Buchner[1], Jihyun Kim[1], and R. Jürgen Behm[1,2] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89081 Ulm, Germany

Here we report results of a UHV study on the interaction of an Ionic Liquid (IL) with lithium on different cobalt oxide thin films as a model study for the solid|electrolyte interphase (SEI) in Li-ion batteries (LIBs). After characterization of CoO(111) and Co_3O_4(111) by X-ray photoelectron spectroscopy (XPS) and scanning probe microscopy, the interaction of ultrathin films of the battery-relevant IL 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide [BMP][TFSI] with Li on CoO and Co_3O_4(111) was investigated, employing mainly XPS. The measurements reveal that intact ion pairs adsorb on both CoO_x surfaces and that postdeposition of Li results in the decomposition of the cations and anions (Li_3N, $LiC_xH_yN_z$, LiF, etc.). In addition, the measurements reveal that Li deposition (both in the presence and absence of an IL adlayer) leads to the conversion of Co^{2+} to Co^0 on CoO and the transformation from Co^{3+} to Co^{2+} on Co_3O_4(111) in the near surface region, due to charge transfer from Li to the surface together with the formation of Li_2O. Hence, the XP spectra resolve the initial stages of the chemical SEI formation (IL decomposition) (in the absence of an applied potential) as well as the reduction of CoO_x, which both play an essential role in the function of LIBs.

O 33.3 Tue 14:30 H10

Trapped electrons and their impact on oxygen reactivity near DMSO/Cu(111) interfaces — •Angelika Demling[1], Sarah B. King[2], Katharina Broch[3], and Julia Stähler[1] — [1]Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]Department of Chemistry and James Franck Institute, University of Chicago, 929 E 57th Street, Chicago, IL 60637, USA — [3]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

DMSO is a common non-aqueous solvent with the potential to be used in lithium-oxygen batteries due to its ability to catalyze superoxide formation [1]. In this study we investigate the electron dynamics in DMSO films on Cu(111) using time- and angle-resolved two-photon photoemission and disentangle the individual steps of charge transfer prior to superoxide formation: Electrons are injected from the metal to the DMSO where they form small polarons on sub-picosecond time scales. The subsequent trapping extends the electronic lifetimes to several seconds [2]. Electron attachment to co-adsorbed O_2 reduces these lifetimes significantly and leads to negative surface charging.
These results highlight the complexity of a standard electrochemical process like superoxide formation.

[1] K. M. Abraham, J. Electrochem. Soc. 162, A3021 (2015)

[2] S. B. King et al., J. Chem. Phys. 150, 041702 (2019)

O 33.4 Tue 14:45 H10

DFT studies on the interface between an ionic liquid and inorganic substrates — •Katrin Forster-Tonigold[1] and Axel Gross[1,2] — [1]Helmholtz Institute Ulm (HIU), Electrochemical Energy Storage, 89069 Ulm, Germany — [2]Ulm University, Institute of Theoretical Chemistry, 89069 Ulm, Germany

In Li-ion batteries the so-called solid|electrolyte interphase (SEI) is formed at the electrode due to decomposition of the electrolyte. As it plays a crucial role for the function of the battery, a thorough understanding of the interface is needed. We employ density functional theory calculations to study the interface between the ionic liquid (IL) 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide used as electrolyte in Li-ion batteries and different inorganic substrates. First, the geometric and electronic adsorption properties of the IL at low coverages and within the monolayer structure at low temperature are discussed [1]. Furthermore, the impact of elevated temperature is taken into account by means of ab initio molecular dynamics simulations. In order to shed some light onto the initial steps of the SEI formation, interactions and reactions between the IL and Li atoms at the interface are considered as well [2].

[1] F. Buchner, K. Forster-Tonigold, M. Bozorgchenani, A. Groß and R. J. Behm. J. Phys Chem. Lett. 7, 226 (2016).

[2] F. Buchner, K. Forster-Tonigold, J. Kim, C. Adler, J. Bansmann, A. Groß and R. J. Behm, J. Phys. Chem. C 122, 18968-18981 (2018).

O 33.5 Tue 15:00 H10

Ion Exchange at the Liquid/Solid Interface in Ultrathin Ionic Liquid Films on Ag(111) — •Matthias Lexow, Bettina Heller, Radha G. Bhuin, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

In the context of ionic liquid (IL) thin film applications, we studied mixed IL systems with respect to surface and interface ion distribution by angle-resolved X-ray photoelectron spectroscopy (ARXPS) as a function of anion, cation, composition, and temperature. By *in-situ* physical vapor deposition, ultrathin layers of two ILs were successively deposited on Ag(111) as model support. By temperature-dependent ARXPS, we found pronounced surface and interface enrichment effects due to rapid ion exchange processes that are proposed to be driven by the interplay of interface adsorption energy and surface free energy in these films.

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

Lexow *et al.*, *ChemPhysChem*, **2018**, DOI: 10.1002/cphc.201800773.

Lexow *et al.*, *Langmuir*, **2018**, submitted.

O 33.6 Tue 15:15 H10

Charge transfer across the GaP(100) photoanode/electrolyte interface during direct, Au-catalysed photoelectrochemical water splitting — •waqas saddique, gerhard lilienkamp, and winfried daum — IEPT, Technical University Clausthal, Clausthal-Zellerfeld, Germany

We have developed a procedure to stabilize n-GaP(100) for operation as a photoanode in hydrochloric acid electrolytes by a thin and dense surface layer of gallium oxide. Here, we report on direct photoelectrochemical water splitting achieved with stabilized photoanodes that, in addition, were functionalized with Au nanoparticles (NPs) as catalysts for water oxidation. The pronounced peaking of the photocurrent at a potential around 0 V vs RHE points to an indirect charge transfer of holes across the semiconductor/electrolyte interface, presumably via defect or interface states with energies in the band gap of GaP. To investigate the charge transfer processes at GaP photoanodes, Nyquist plots were measured for different applied potentials by electrochemical impedance spectroscopy, and reproduced by simulations with an appropriate equivalent electrical circuit. The plots reveal minimum impedance at a potential of -0.05 V vs RHE, which coincides with the exact potential of maximum photocurrent in cyclic voltammetry. The Nyquist plots are composed of 6 (!) semi-circles, and their specific potential dependence reveals unprecedented details of a 6-step charge transfer process that includes all four steps of the water oxidation reaction. Our results highlight the favourable electrocatalytic properties of Au-NPs for all intermediate steps of the water oxidation reaction.

O 33.7 Tue 15:30 H10

Semiconductor/water interfaces: ab initio molecular dynamics at constant electrode potential and spectroscopic signatures — •Stefan Wippermann[1], Lei Yang[2], Fang Niu[1], Marc Pander[1], Andreas Erbe[3], Mira Todorova[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, Germany — [2]Kanazawa University, Japan — [3]NTNU Trondheim, Norway

Despite the importance of understanding the structural and bonding properties of solid-liquid interfaces for a wide range of (photo-)electrochemical applications, there are presently no experimental techniques available to directly probe the microscopic structure of solid-liquid interfaces. To develop robust strategies to interpret experiments and validate theory, we carried out attenuated total internal reflection (ATR-IR) spectroscopy measurements and ab initio molecular dynamics (AIMD) calculations for interfaces between liquid water and well-controlled prototypical semiconductor substrates. The calculations are performed at constant electrode potential, based on the approach recently suggested by S. Surendralal et al. [1]. We discuss interactions between commonly used thermostats and the potentiostat, and suggest to introduce temperature-induced dipole fluctuations directly into the potentiostat scheme. This new approach has been validated by extensive benchmarks and is shown to not affect the vibrational spectra at the solid-liquid interface. Support from BMBF NanoMatFutur grant No. 13N12972 is gratefully acknowledged.

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

O 33.8 Tue 15:45 H10

Two-dimensional Polymer Structures for Energy Conver-

sion — •Patrick Alexa[1], Doris Grumelli[2], Juan Lombardi[3], Paula Abufager[3], Heriberto Busnengo[3], Vijay Vyas[1], Frederik Haase[1], Bettina Lotsch[1,4], Rico Gutzler[1], and Klaus Kern[1,5] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Universidad Nacional de La Plata, Argentina — [3]Universidad Nacional de Rosario, Argentina — [4]University of Munich (LMU), Germany — [5]Ecole Polytéchnique Fédérale de Lausanne, Switzerland

During the last decade the necessity for clean and renewable energy sources has driven societal and political agendas. Progress in energy conversion chemistry can be achieved by the utilization of tailored nanomaterials created in a bottom-up approach, for example when used as efficient electrocatalysts. In this work we investigate two-dimensional networks for their propensity for the hydrogen evolution reaction. In particular, we synthesize two-dimensional polymers with varying amount of nitrogen heteroatoms on Au(111) and visualize their topography by scanning tunneling microscopy. The polymer decorated surface shows promising enhancement effects for the catalytic activity of the hydrogen evolution reaction. The influence of the electrochemical conditions on the organic structure is discussed as well as the varying nitrogen content on electrocatalytic activity. The experimental and theoretical results highlight the capability of single-layer functional two-dimensional polymers for electrocatalysis and provide a molecular picture that explains increased catalytical activity.

O 33.9 Tue 16:00 H10

Theoretical study of two-dimensional titanium carbide MXenes functionalization process — •Rina Ibragimova, Martti Puska, and Hannu-Pekka Komsa — Aalto University, Espoo, Finland

MXene phases are a new rapidly developing class of two-dimensional materials with suitable electronic, optical and mechanical properties for different applications. These phases consist of transition metals such as Ti, Sc, Zr, Hf, V, Nb, Ta, Cr, Mo and carbon or nitrogen atoms, and can be produced through the etching of layered MAX phases. During the etching process, it is possible to terminate the surface by O, OH, and F functional groups in order to modify materials properties. In this work, we accurately describe the surface distribution of functional groups and its interaction with Ti-based two-dimensional carbides in the solution through the use of different approaches. The free Gibbs energies of formation for the distinctly terminated surfaces have studied by combining DFT, phonon calculations and implicit solvation model. Our results indicate the formation of O, OH and F mixture, which coincides with experimental data. Furthermore, DFT together with cluster expansion (CE), and Monte Carlo methods are employed to investigate the distribution of the functional groups on the surface. The proposed computational approach allows us to deeper understand a functionalization mechanism and introduce the range of experimental conditions for further tuning the MXenes properties.

O 34: New Methods and Developments III: Spectroscopy and Tribology

Time: Tuesday 14:00–15:45 Location: H13

O 34.1 Tue 14:00 H13

Atomic Scale Structure and Frictional Response of Swift Heavy Ion Irradiation Induced Defects on Graphitic Surfaces — •Dilek Yildiz[1,2], Cem Kincal[1], Umut Kamber[1], Cornelis J. van der Beek[3], and Oguzhan Gürlü[1] — [1]Istanbul Technical University, Department of Physics, 34460, Istanbul, Turkey — [2]University of Basel, Department of Physics, Basel, Switzerland — [3]Ecole Polytechnique, Palaiseau, France

Hillock and comet-like structures on swift heavy ion (SHI) irradiated highly oriented pyrolytic graphite (HOPG) surfaces were previously reported. It was shown that chains of hillocks were formed on HOPG due to SHI irradiation under grazing incidence. Using Scanning Tunneling Microscopy (STM) we have obtained atomic resolution on the tail sections of the comets as well as on the chains forming around them. Such data indicates that the interaction of SHI with the bulk of HOPG damages the atomic order on the surface layer only locally. SHI irradiation induced corrugation changes on flat surfaces can be imaged by STM to a certain extent. Friction force microscopy showed complementary results. We have observed that the tail sections of the comets appeared on friction maps, although they could not be seen in simultaneously taken contact mode AFM topography images. Our data on SHI irradiation of moire zones that formed due to rotated graphene layers on HOPG surfaces indicate that the structure of the SHI induced defects on graphene/HOPG system varies due to local conductivity differences between moire zones.

O 34.2 Tue 14:15 H13

Ultrasensitive charge detection to study contact electrification between a steel ball and a gold surface — •Andre Mölleken, Hüseyin Azazoglu, Doris Tarasevitch, Tobias Roos, Detlef Utzat, Hermann Nienhaus, and Rolf Möller — Fakultät für Physik/Cenide, Universität Duisburg-Essen, Germany

Contact electrification and charge transfer between particles in granular matter are of high technological and fundamental interest. As a model system, we have studied the free fall of a single steel ball of 1mm in diameter on a gold coated copper plate of a parallel plate capacitor. The ball hits the surface with an initial velocity of approximately 0.6m/s and bounces afterwards repeatedly on the surface. If the moving steel ball is charged it creates an image charge in the plate which is measured as a function of time. The induced and the transferred charge is measured using an extremely sensitive and fast charge detector [1], capable of detecting a few thousand elementary charges with a 50 kHz bandwidth. Kinetic parameters and energy transfer coefficients can be extracted from the data. In addition, the charge transfer between ball and plate is precisely determined for every collision. Different kinds of charge transfer are found, e.g., reduction and increase of the charge on the ball as well as polarity changes. A complete discharging as expected for a metallic contact occurs only very rarely. However, there is a significant tendency that the charges before and after collision are related to each other and the total amount of transferred charge correlates with the impact velocity. [1] P. Graf. et al., Rev. Sci. Instrum. 88, 084702 (2017).

O 34.3 Tue 14:30 H13

Nano-scale surface steps as the origin of friction anisotropy of snake scales — •Weibin Wu[1], Shudong Yu[2], Christian Greiner[3], Guillaume Gomard[1,2], and Hendrik Hölscher[1] — [1]Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT) — [2]Light Technology Institute (LTI), Karlsruhe Institute of Technology (KIT) — [3]Institute for Applied Materials (IAM), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Snakes exhibit special locomotion styles because they are legless and slide in direct contact with the ground. Therefore, their ventral scales feature interesting tribological properties. Previous studies analyzed oriented micron-sized fibril structures on the scales which seem beneficial for controlling friction during sliding but the actual nano-scale interaction mechanism was rarely explained. We characterized the friction behavior of this fibril structure by AFM and measured friction while scanning the step edges of the fibrils up and down. The mirco-fibril structures on the ventral scale of snakes produce comparable large friction peaks during upward scans but considerable lower friction for downward scans. This behavior leads to friction anisotropy in the direction of locomotion. The same result is found for the dorsal scales of sandfish (Scincus scincus) and a polymeric replica of scales of the Chinese cobra (Naja atra). The overall effect increases linearly with step height. Although different snake species exhibit diverse step heights, the distribution of step heights along the body of the examined snakes is very similar indicating dedicated friction anisotropy in different sections along snake bodies.

O 34.4 Tue 14:45 H13

surface characterization of ruthenium as novel barrier layer during the chemical mechanical polishing process of integrated circuit for sub-10 nm technology node — •jie cheng[2], xinchun lu[1], and jinshan pan[2] — [1]state key lab of tribology, tsinghua university, beijing, china — [2]division of surface and corrosion science, kth royal institute of technology, Stockholm, Sweden

Ruthenium (Ru), as a novel diffusion barrier layer, is quite promising in the application of the sub-10 nm technology node of integrated circuit. During the chemical mechanical polishing process of Ru, complex changes will occur on Ru surface and Cu/Ru interface under the function of both mechanical abrasion and the chemical corrosion. This paper focuses on the study of surface properties of Ru in potassium periodate solutions: chemical and physical properties of surface films on Ru such as thickness, compactness, uniformity, and chemical compositions; tribology and corrosion properties of Ru like corrosion, galvanic corrosion (between Ru and Cu), and tribo-corrosion during the abrasion process. On this basis, the material removal mechanism of Ru is fully revealed during the chemical mechanical polishing process, the technique of which is widely used to realize local and global planarization of wafer surfaces. Results explores the nature of tribo-corrosion: the galvanic corrosion between the abrasion induced depassivation area and the passivation area. The evolution of three periodical changes between Ru and Cu interface was also fully revealed by microscopic methods. The findings in the research have guiding significance to the smooth application of Ru as substitutive barrier layer.

O 34.5 Tue 15:00 H13

Projection Analysis of EXAFS Modulations — Alireza Bayat[1], Angelika Chassé[1], Reinhard Denecke[2], Stefan Förster[1], Paula Huth[2], Eva-Maria Zollner[1], and •Karl-Michael Schindler[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut f. Physik, D-06099 Halle, Germany — [2]Wilhem-Ostwald-Institut f. Physikalische und Theoretische Chemie, D-04103 Leipzig, Germany

EXAFS modulations have been analysed using a direct projection method known from structure determinations using photoelectron diffraction [1]. In this method experimental EXAFS modulations are projected onto calculated ones with just one singular neighbouring atom at a series of distances. Compared to the usual analysis with a Fourier transform of the EXAFS modulation function, the systematic errors in initial values for nearest neighbor distances are significantly reduced from 40 - 80 pm to below 10 pm. This improvement results from the correct treatment of the energy dependence of the phase shift within the scattering process at the neighboring atom. Tests of the method are presented with experimental EXAFS modulations from strontium titanate and barium titanate single crystals as well as from a newly discovered barium titanate derived quasicrystalline film on a Pt(111) substrate [2].

References:
[1] P. Hofmann and K.-M. Schindler, Phys. Rev. B 47, 13941 (1993).
[2] S. Förster et al., Nature 502, 215 (2013).

O 34.6 Tue 15:15 H13

Removing Photoemission Features from Auger-yield NEXAFS Spectra — •Ole Lytken, Daniel Wechsler, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg

Auger-yield is widely used for surface-sensitive NEXAFS measurements, but suffers from errors introduced by photoemission features travelling through the measured Auger peaks. We will present two-dimensional NEXAFS images, measured at the Materials Science beamline at Elettra in Trieste, and a procedure for removing the photoemission features travelling through the images. The procedure relies on describing the measured Auger-yield NEXAFS images as three simple, one-dimensional spectra: NEXAFS, Auger and XPS, which are extracted through an iterative process. The procedure requires no additional reference measurements other than photon flux and the success of the cleanup process is easily verified by the resulting images.

O 34.7 Tue 15:30 H13

New reconstruction method for Metastable Induced Electron Spectra of molecules on solid surfaces — •Tobias B. Gäbler, Wichard J. D. Beenken, and Erich Runge — Technische Universität Ilmenau, Institute for Physics, Ilmenau, Germany

The Metastable Induced Electron Spectroscopy (MIES) allows an extremely sensitive electronical characterization of liquid and solid surfaces by deexcitation of metastable rare gas atoms. We present ab initio calculations of MIES spectra of molecules physisorbed on solid surfaces. For this purpose, we calculate spatially distributed transition rates of the Auger deexcitation process without the simplifying assumptions as proposed by Kantorovich et al. [1]. Thereby, we model the density of metastable Helium atoms along a series of trajectories approaching the sample molecule. According to experimental results for benzene [2], our calculations demonstrate - in contrast to the approach of Kantorovich et al. [1] - an anisotropy of the MIES spectra in respect not only to the molecule orientation but also to the electron detection direction. Thus, due to the ajustable direction of the incidence of metastable helium and of the detection of emitted Auger-electrons in the simulation, our method is able to forecast MIES spectra for arbitrary experimental setups.

[1] L.N. Kantorovich, A.L. Shluger, P.V. Sushko, A.M. Stoneham, Surf. Sci. 444 (2000) 31-51
[2] J. Günster, G. Liu, V. Kempter, D.W. Goodman, Surf. Sci. 415 (1998) 303-311

O 35: 2D Materials I: Growth and Properties of Transition Metal Dichalcogenides, Phase Transitions

Time: Tuesday 14:00–16:45 Location: H14

O 35.1 Tue 14:00 H14

The unoccupied electronic structure of 2H tungsten disulfide — •Lukas Musiol, Philipp Eickholt, and Markus Donath — Westfälische-Wilhelms-Universität Münster, Germany

In the field of 2D materials, single-layer transition metal dichalcogenides, especially MoS_2, WS_2, $MoSe_2$, and WSe_2, play an important role. Due to their exceptional optical and electronic properties, they are promising materials for optoelectronical applications. The key to understanding the material properties is a profound knowledge of the electronic structure. Because freestanding single layers cannot be prepared, experiments are conducted on single layers deposited on a substrate. While the spin structure of the occupied and unoccupied K valleys was investigated for WS_2/Au(111) [1], the influence of the Au(111) substrate is not known in detail.

We present an angle-resolved inverse-photoemission [2,3] study of 2H-WS_2. By comparison with data of single-layer WS_2/Au(111), the influence of the Au(111) substrate is extracted.

[1] P. Eickholt *et al.*, Phys. Rev. Lett. **121**, 136402 (2018)
[2] M. Budke *et al.*, Rev. Sci. Instrum. **78**, 113109 (2007)
[3] S.D. Stolwijk *et al.*, Rev. Sci. Instrum. **85**, 013306 (2014)

O 35.2 Tue 14:15 H14

Charge-transfer across the $MoSe_2$/WSe_2 interface studied with second-harmonic imaging microscopy — •Jonas E. Zimmermann, Ulrich Höfer, and Gerson Mette — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, 35032 Marburg

2D transition metal dichalcogenides (TMDC) have been in the center of attention since the discovery of extraordinary luminescence for MoS_2. TMDC heterostructures in particular gain more and more popularity due to their possible applications in optoelectronics. As the efficiency of such devices is expected to depend strongly on the charge transfer across the heterointerface, it is of crucial importance to investigate the charge-carrier dynamics on a fundamental level.

Here we present results of our second-harmonic (SH) imaging microscopy setup for time-resolved studies on interfaces of 2D materials. This technique enables us to quantify the crystal orientation via polarization dependent measurements and at the same time provides access to the charge-carrier dynamics by femtosecond pump-probe experiments. Measurements performed on MoS_2 monolayers show a strong pump-induced change in the SH response which corresponds well to the fingerprint of exciton generation reported for this material. In contrast, experiments on a $MoSe_2$/WSe_2 heterostructure reveal a delayed filling as well as an enhanced lifetime of the temporal signature. These findings suggest the generation of interlayer excitons in the heterostructure.

O 35.3 Tue 14:30 H14

Phonon dispersion of bulk MoS_2 determined by high resolution electron energy loss spectroscopy — •Holger Schwarz, Christian Heidrich, Florian Speck, and Thomas Seyller — Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126

Chemnitz, Germany

Transition metal dichalcogenides are currently receiving considerable interest because they are considered as potential building blocks for novel device architectures made up from 2D materials. Basic properties like, e.g. electronic structure as well as phonon and plasmon dispersion, are of fundamental interest in this respect. High resolution electron energy loss spectroscopy (HREELS) is a powerful tool for the investigation of the phononic structure of a solid. Here we use HREELS to study the phonon dispersion of molybdenum disulfide (MoS_2). A clean surface of a MoS_2 bulk crystal was prepared by mechanical cleavage and mild annealing in ultra-high vacuum (UHV). Using low-energy electron diffraction (LEED), the sample was aligned in the high symmetry directions Γ-K and Γ-M, respectively, and subsequent HREELS measurements have been performed in off-specular geometry with a fixed incident electron energy and angle by varying the detector angle of the spectrometer. The spectra were fitted using Voigt-profiles for each resolvable phonon mode. The results are in good agreement with recent DFT-calculations from literature [1] but certain differences in comparison to an earlier HREELS study [2] were noted. [1] A. Molina-Sánchez and L. Wirtz, Phys. Rev. B 84, 155413 (2011) [2] P. A. Bertrand, Phys. Rev. B 44, 5745 (1991)

O 35.4 Tue 14:45 H14

Composition dependence of charge driven phase transition in Group-VI transition metal dichalcogenides from first-principles — Urvesh Patil and •Nuala Mai Caffrey — School of Physics & CRANN, Trinity College, Dublin 2

Atomic intercalation can induce structural phase transitions in a host layered material. For example, group-VI transition metal dichalcogenides (TMDs) are known to undergo a charge-induced phase transition from a semi-conducting H-phase to a metallic T′-phase [1]. The ability to control this phase transition would be advantageous for 2D electronics and catalysis, but it is not well understood, particularly for TMDs beyond MoS_2. Experiment has found that it is comparatively difficult to induce this phase transition in MoS_2 compared to WS_2. However, it is not understood if this can be attributed directly to the electronic properties of these materials, or if the production technique indirectly controls it [2].

Here, we perform a comprehensive side-by-side first-principles investigation of group-VI TMDs (MX_2, where M = Mo, W and X = S, Se), aimed at understanding how alkali metal adsorption affects the phase transition. We show that the barrier for MoS_2 conversion is indeed significantly higher than that of the other TMDs. Finally, we discuss how structural distortions affect the stability of the metallic phase.

[1] Voiry et al, Chemical Society Reviews **44** 2702 (2015)

[2] Ambrosi et al, Chemical Communications **51** 8450 (2015)

O 35.5 Tue 15:00 H14

Observing different levels of airborne contaminations on TMDC materials — •Korbinian Pürckhauer, Dominik Kirpal, Alfred J. Weymouth, and Franz J. Giessibl — University of Regensburg, Regensburg, Germany

The development in nanoelectronics demands reducing the size of its elements which led to an increase of interest in TMDCs. These show a range of interesting properties like a band gap in the range of Si and GaAs and allow high on/off switching ratios for FETs. Fabrication of devices incorporating those TMDCs is mostly done in ambient conditions and thus investigation of TMDCs in ambient is sustainable for the future. We imaged MoS_2, WS_2, $MoSe_2$ and WSe_2 in real space by using atomic force microscopy (AFM). Mechanical exfoliation of the TMDCs provided very large (at least hundreds of nm) clean terraces on MoS_2 and WS_2. In contrast, the $MoSe_2$ and WSe_2 surfaces appeared to be contaminated directly after cleavage in most cases. On all surfaces we were able to observe atomic resolution in ambient conditions. Our findings suggest that TMDCs with sulfur as a chalcogen atom are more suitable for devices made in ambient conditions.

O 35.6 Tue 15:15 H14

Unraveling the growth mechanism of single-domain molybdenum disulfide on Au(111) — •Moritz Ewert[1,2,3], Lars Buss[1,3], Paolo Moras[4], Jens Falta[1,2], and Jan Ingo Flege[1,2,3] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Germany — [3]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [4]Istituto di Struttura della Materia del Consiglio Nazionale delleRicerche, Sincrotrone Trieste SCpA, Italia

As a transition metal dichalcogenide single-layer molybdenum disulfide (MoS_2) is a heavily investigated system. Due to its direct band gap, the electronic properties of single-layer MoS_2 have been subject to several surface science methods. A well-known model system is MoS_2 on Au(111).

We present in situ low-energy electron microscopy (LEEM) and micro-diffraction (LEED) observations of MoS_2 growth on Au(111) at elevated temperature using two distinctly different deposition rates. Our investigations reveal similar but different expansion mechanisms of the MoS_2 islands changing a balanced distribution of the two mirror domains towards a single domain distribution. Structural characterization by I(V)-LEEM and investigations of the electronic bandstructure using angle-resolved photoelectron spectroscopy both confirm single-layer nature of the MoS_2 islands. We could identify step pushing of the growing MoS_2 being responsible for this phenomena.

O 35.7 Tue 15:30 H14

Controlled growth of transition metal dichalcogenide monolayers using Knudsen-type effusion cells for the precursors — •Antony George[1], Christof Neumann[1], David Kaiser[1], Rajeshkumar Mupparapu[1], Tibor Lehnert[2], Uwe Hübner[3], Zian Tang[1], Andreas Winter[1], Ute Kaiser[2], Isabelle Staude[1], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena, Germany — [2]Ulm University, Central Facility of Materials Science Electron Microscopy, 89081 Ulm, Germany — [3]Leibniz Institute of Photonic Technology, 07745 Jena, Germany

Controlling the flow rate of precursors is essential for the growth of high quality monolayer single crystals of transition metal dichalcogenides (TMDs) by chemical vapor deposition. Thus, introduction of an excess amount of the precursors affects reproducibility of the growth process and results in the formation of TMD multilayers and other unwanted deposits. Here we present a simple method for controlling the precursor flow rates using the Knudsen-type effusion cells. This method results in a highly reproducible growth of large area and high density TMD monolayers. The size of the grown crystals can be adjusted between 10 and 200 μm. We characterized the grown MoS_2 and WS_2 monolayers by optical, atomic force and transmission electron microscopies as well as by Raman and photoluminescence spectroscopies, and by electrical transport measurements showing their high optical and electronic quality based on the single crystalline nature.

O 35.8 Tue 15:45 H14

Reversible crystalline-to-amorphous phase transition in MoS_2 on Gr/Ir(111) by ion irradiation — •Philipp Valerius[1], Joshua Hall[1], Silvan Kretschmer[2], Mahdi Ghorbani-Asl[2], Alexander Grüneis[1], Arkady V. Krasheninnikov[2,3], and Thomas Michely[1] — [1]Universität zu Köln, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]Aalto University, Finland

Grazing incidence 500 eV Xe^+ irradiation transforms a crystalline monolayer of MoS_2 resting on Gr/Ir(111) into an amorphous material as shown by LEED and STM measurements. Moreover, a significant density of states in the band gap evolve, which is evidenced by scanning tunneling spectroscopy. Molecular dynamics simulations uncover that under the irradiation conditions used, sulfur is selectively removed from the top layer, while Mo and the bottom S layer is not sputtered. Through annealing in S vapor, the MoS_2 can be restored as a crystalline semiconductor close to perfection. The structural phase transitions are accompanied by changes in the Raman modes and photoluminescence. As the amorphized MoS_2 monolayer displays metallic properties, selective ion beam amorphization of contact areas could be used as a method to avoid Schottky barriers when contacting MoS_2.

O 35.9 Tue 16:00 H14

Damage mechanisms in two-dimensional MoS_2 under electron irradiation — •Silvan Kretschmer[1] and Arkady Krasheninnikov[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Applied Physics, Aalto University School of Science, Aalto, Finland

Two-dimensional (2D) materials are routinely characterized nowadays in the transmission electron microscope (TEM). The high-energy electron beam in TEM can create defects in the target, and as the influence of defects on materials properties is expected to be stronger in systems with reduced dimensionalities, understanding defect production in 2D materials is of particular importance. Irradiation-induced defects can appear through three mechanisms, namely ballistic or knock-on damage (1), ionization and electronic excitations (2) and beam-induced chemical etching (3). Only the first channel is well understood, while observations of defects formation in 2D transition metal dichalcogenides below the knock-on threshold points out that other mechanism should be important. Here we investigate the role of electronic excitations in defect production by using advanced first-principles simulation techniques based on the Ehrenfest dynamics combined with time-dependent density-functional theory and demonstrate that a combination of excitations and knock-on damage in 2D MoS2 under electron beam can give rise to the formation of vacancies and explain the experimental observations.

O 35.10 Tue 16:15 H14

Nano-patterning of MoS_2 monolayers with focused ion beam — •Rajeshkumar Mupparapu[1], Michael Steinert[1], Antony George[2], Franz Löchner[1], Zian Tang[2], Tobias Bucher[1], Frank Setzpfandt[1], Andrey Turchanin[2], Thomas Pertsch[1], and Isabelle Staude[1] — [1]Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena, Germany

Monolayers of transition metal dichalcogenides (TMD-MLs) are immensely interesting for their versatile emission properties [1]. Typically, emission of these extremely thin materials is manipulated either by integrating them on to nanostructures or by assembling into heterostructures. Nano-patterning of TMD-MLs into desired shapes and sizes adds another degree of freedom for their emission manipulation [2, 3]. In this work, we report on nano-patterning of MoS_2 monolayers (MoS_2-MLs) with focused gallium-ion beam while minimizing the damage to the MoS_2 material. To investigate the influence of nano-patterning on emission properties of MoS_2-MLs, we performed photoluminescence, Raman and second harmonic generation measurements. References: [1]. Q. Wang et al., Nat. Nanotech., 7, 699-712 (2012). [2]. W. Guohua et al., Sci. Rep., 7, (2017). [3]. J. Yang et al., Light Sci. Appl., 5, e16046 (2016).

O 35.11 Tue 16:30 H14

Towards Molecular-level Understanding of Ice Nucleation Inhibition at Surfaces — •Naureen Akhtar — Department of Physics and Technology, University of Bergen, P.O. Box 7803, N-5020, Bergen, Norway

The paper that I here submit for the Gerhard Ertl Young Investigator Award presents the first experimental study of the anti-icing properties of graphene and functionalized graphene (fluorinated). The paper demonstrates a completely new approach to anti-icing surfaces, defining a new class of materials, where anti-icing is achieved solely by structuring on the atomic level. The results presented in the paper demonstrate excellent anti-icing performance with freezing delays up to several hours in a high humidity environment. It presents a realistic anti-icing solution that can be implemented in practice. Furthermore the research presented in the paper introduces graphene as a new model-system for understanding ice nucleation mechanism. Finally the results and further work with this new class of material may contribute to the improvement of climate models through the understanding of the role of ice formation in clouds via seeding materials. This is because soot particles are ubiquitous aerosols in the atmosphere and graphene derivatives may serve as suitable model systems, ultimately providing data that can be incorporated in climate models where these effects are currently not taken into consideration.

O 36: Focus Session: Designer Quantum Systems II (joint session O/TT)

Time: Tuesday 14:00–15:45 Location: H15

Invited Talk O 36.1 Tue 14:00 H15

Topological quantum phases in atomically precise graphene nanoribbons — •Oliver Gröning[1], Shiyong Wang[2], Qiang Sun[1], Akimitsu Narita[3], Müllen Klaus[3], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa Materials Science and Technology, Dübendorf, Switzerland — [2]School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai, China — [3]Max Planck Institute for Polymer Research, Mainz, Germany

Topological materials have attracted great interest in solid state physics due to their ability to support robust, yet exotic quantum states at their boundaries or interfaces such as spin-momentum locked transport channels or Majorana fermions. Very recently, it has been found theoretically by Louie et al., that localized zero energy modes can be obtained at the junctions of topologically dissimilar graphene nanoribbons (GNR). We have experimentally realized such GNR junctions using on-surface synthesis, i.e. by the polymerization of molecular precursors rationally designed to yield the desired final GNR on single crystal surfaces. By creating well defined periodic sequences of these topological electronic modes, one-dimensional electronic bands can be created, which are described by the Su-Schrieffer-Heeger (SSH) Hamiltonian representing the dimerized atomic chain. By manipulating the intra- and inter-cell coupling strength we could further create SSH analogs with different winding number and therefore topological class. The topological class distinction is evidenced by presence, respectively absence of zero energy end states at the termini of the corresponding GNR or their junctions to structurally dissimilar GNRs.

Invited Talk O 36.2 Tue 14:30 H15

Electronic properties of twisted graphene layers: bands, interactions and superconductivity. — •Francisco Guinea — Imdea Nanscience, Faraday , 28049 Madrid, Spain — School of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK

Twisted graphene bilayers show an unusual band structure, with very narrow bands. In these bands, states with different momenta show significant variations in their charge density. A change in the number of carriers leads to inhomogeneous charge distributions, which, in turn, modify significantly the shape of the bands. This effect can be described in terms of emergent assisted hopping interactions. These couplings tend to favor superconductivity.

O 36.3 Tue 15:00 H15

Symmetry breaking in Molecular Artificial Graphene — •Linghao Yan[1,2], Muqing Hua[2], Qiushi Zhang[2], Tsz Ue Ngai[2], Zesheng Guo[2], Tsz Chun Wu[2], Tong Wang[2], and Nian Lin[2] — [1]Aalto University, Finland — [2]The Hong Kong University of Science and Technology, Hong Kong, China

Artificially-assembled molecular lattices on metal surfaces, known as molecular designers (Nature 483, 306, 2012), have been used as simulators to explore exciting physics that are extremely challenging to access in real materials. For example, gauge field, edge states and flat band are demonstrated in artificial grahpene, graphene nanoribbons, and Lieb lattice. In this work, we exploit the unique tunability of the molecular designers to break the symmetry of Dirac quasiparticles. The importance of symmetry breaking in graphene for applications has been widely recognized. Several schemes have been proposed, including breaking sublattice symmetry and applying uniaxial strain. Here we report the realization of both of these schemes by designing isotropic molecular potentials and isotropic lattices, respectively. The spatially-resolved local density of states acquired using scanning tunneling spectroscopy confirm that in both cases the local density of states undergo characteristic changes.

O 36.4 Tue 15:15 H15

On-Surface Synthesis and Characterization of Cycloarenes: a C108 Graphene Quantum Ring — •Qitang Fan[1], Daniel Martin Jimenez[2], Simon Werner[1], Daniel Ebeling[2], André Schirmeisen[2], Jörg Sundermeyer[1], Wolfgang Hieringer[3], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Institute of Applied Physics (IAP), Justus Liebig University Gießen, Germany — [3]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Cycloarenes, such as kekulene, are a unique class of polycyclic aromatic hydrocarbons (PAHs). They enclose a cavity by circularly annulated benzene rings. In a modern view, they can thus be considered as nanorings cut-out from graphene with atomic precision. These graphene rings could serve as useful model quantum materials for the exploration of geometry-dependent electronic properties of nanographenes, e.g., the Aharonov-Bohm effect in graphene quantum rings. However, the synthesis and characterization of cycloarenes with more than one band of benzene rings is still challenging due to their special ring-shaped geometry and low solubility. Here, we employed the high-dilution principle both on a metal surface and in solution to synthesize a novel hexagonal cycloarene with two bands of annulated benzene rings, containing 108 sp2 carbons, by hierarchical Ullmann coupling and cyclodehydrogenation reaction of dibrominated aromatic precursors. The structure and properties of this C108 cycloarene molecule has been unambiguously clarified by various techniques including STM/STS, nc-AFM, UV-vis spectroscopy, and DFT calculations.

O 36.5 Tue 15:30 H15

Nonlinear optical Hall effect in BC_2N — •Julen Ibañez-Azpiroz[1], Ivo Souza[1,2], and Fernando de Juan[2,3] — [1]Materials Physics Center, CSIC-UPV/EHU, 20018 Donostia-San Sebastián, Spain — [2]Ikerbasque Foundation, 48013 Bilbao, Spain — [3]Donostia International Physics Center (DIPC), 20018 Donostia, Spain

The bulk photovoltaic effect is a nonlinear optical response that yields a net photocurrent in noncentrosymmetric crystals. Its interband contribution under linearly polarized light, known as the *shift current*, involves a subtle Berry-phase-like quantity that makes this effect very sensitive to wavefunction properties. Here we show that the relative parity of valence and conduction bands under mirror reflection determines whether the shift current flows parallel or perpendendicular to the applied electric field. The former situation is realized in GeS and similar monolayers [1,2] while the later, which corresponds to a nonlinear optical Hall effect, is far less common. Based on a recently developed *ab-initio* method [3], we show that this novel effect is realized in layer-structured graphitic BC_2N. Furthermore, our calculations reveal an enhanced shift-current absorption in the visible range, which makes BC_2N a prime candidate for future experimental studies.

[1] A. Cook, B. M. Fregoso, F. de Juan et. al., Nat. Commun. **8**, 14176 (2017).

[2] T. Rangel, B. M. Fregoso, B. S. Mendoza et. al., Phys. Rev. Lett. **119**, 067402 (2017).

[3] J. Ibañez-Azpiroz, S. S. Tsirkin and I. Souza, Phys. Rev. B **97**, 245143 (2018)

O 37: Metal Oxide Surfaces II: Structure, Epitaxy and Growth

Time: Tuesday 14:00–16:45 Location: H16

O 37.1 Tue 14:00 H16

Growth and phase transitions of wurtzite CoO films on Au(111) — •Maximilian Ammon[1], Sara Baumann[1], Tilman Kisslinger[1], Lutz Hammer[1], Josef Redinger[2], and M. Alexander Schneider[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058, Germany — [2]Institut für Angewandte Physik & CMS, TU Wien

The metastable wurtzite polymorph of CoO shows interesting properties, but has so far only be found as nanoparticles and islands on Au(111) [1,2]. Here we establish the wurtzite polymorph on Au(111) by a LEED-I(V) analysis, STM and DFT calculations.

Cobalt oxide films with a thickness of ∼ 3 nm are grown reactively on Au(111) at T = 280 K in UHV. STM identifies that films grown under oxygen poor conditions are closed with grain sizes around 20 nm. LEED-I(V) proves the structure to be oxygen-terminated wurtzite CoO ($R_P = 0.13$), the structural parameters are in agreement with DFT calculations. Oxygen rich conditions lead instead to spinel Co_3O_4. Both polymorphs undergo distinctly different irreversible phase transitions upon annealing in UHV: wurtzite CoO is a precursor for rocksalt CoO(100) ($T \geq 600$ K), while spinel CoO converts above 800 K to rocksalt CoO(111). Films of a thickness $\lesssim 1$ nm grow only in the wurtzite phase as identified by the conversion to CoO(100) and the observed lattice constant of 0.326 nm.

[1] Risbud et al., Chem. Mater. 17, 834-838 (2004)

[2] Walton et al., ACS Nano 9, 2445-2453 (2015)

O 37.2 Tue 14:15 H16

Dopant-induced diffusion at metal-oxide interfaces studied for Fe- and Cr-doped MgO/Mo(001) films — Stefania Benedetti[1], Sergio Tosoni[2], Gianfranco Pacchioni[2], and •Niklas Nilius[3] — [1]CNR, Instituto Nanoscienze, 41125 Modena, Italy — [2]Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, 20125 Milano, Italy — [3]Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany

X-ray photoelectron spectroscopy reveals spontaneous atom diffusion from a Mo(001) support into a MgO thin film doped with transition-metal ions. The amount of interfacial mixing depends on the nature of the dopants and is larger for Fe than for Cr impurities. DFT calculations find the reason for Mo diffusion in the ability of the dopants to change oxidation state. Cr exclusively occurs as 3+ ion in MgO and charge mismatch with native ions is compensated for by Mg vacancies. Conversely, the Fe oxidation state depends on temperature, which enables Mo atoms from the support to move into Mg vacancies where they oxidize via electron transfer into the Fe dopants. The talk unravels a novel charge-compensation scheme in doped oxides that proceeds via chemical intermixing at a metal-oxide interface.

O 37.3 Tue 14:30 H16

High quality MgO-films grown at low temperatures on CoO(100) — •Alexandra Schewski, Tilman Kisslinger, Lutz Hammer, and Alexander Schneider — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg

Interfaces between oxides have recently received great attention showing that new electronic properties [1] but also an influence on magnetic transition temperatures can be observed, e.g. for rocksalt CoO on Fe_3O_4[2]. In all these cases it is important to prepare a high quality interface and ideally characterize its structure.

Here we report on the growth and characterization of the non-magnetic insulator MgO on the anti-ferromagnet CoO. As a substrate we used CoO(100) films on Ir(100) that grow perfectly with terrace sizes larger than 200 nm [3]. On top, we deposited Mg reactively in an oxygen atmosphere at different temperatures and subsequently annealed up to a maximum of 1270 K. Surprisingly, even low-temperature deposition at 90 K leads to well-ordered, closed films with a sharp (1×1) LEED-pattern. The LEED-I(V) analysis confirms pure MgO(100) overlayers. It is remarkable that the film quality does hardly improve by annealing up to 870 K. Annealing beyond this temperature leads to the recovery of the CoO(100) LEED-pattern due to a dewetting of the MgO on the surface. The formed micrometer sized MgO particles on CoO are readily identified by SEM.

[1] F. Hellmann et al. Rev. Mod. Phys., **89**, 025006 (2017).

[2] Y. Ijiri et al. , Phys. Rev. Lett. **99**, 147201 (2007).

[3] K. Heinz, L. Hammer, J. Phys.-Condens. Mat. **25** 173001 (2013)

O 37.4 Tue 14:45 H16

EuO ultrathin films: Growth and strain engineering — •Paul Rosenberger[1], Patrick Lömker[2], and Martina Müller[1,3] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, Jülich — [2]Deutsches Elektronen-Synchrotron (DESY), Hamburg — [3]Expt. Physik I, TU Dortmund, Dortmund

It has been shown that the ferromagnetic insulator Europium monoxide (EuO) is a highly efficient spin filter and thus a very interesting material for spintronics. Furthermore, EuO is predicted to become ferroelectric, and thus multiferroic, under sufficiently large biaxial strain. Our goal is to synthesize ultrathin strained EuO films onto suitable substrates and to study their electronic and magnetic properties.

We grow EuO (ultra-)thin films ($d \lesssim$ 10ML) using MBE in an adsorption-limited growth mode, which is typically employed to synthesize stoichiometric films free from metallic Eu or its higher oxides. We use Yttria-stabilized zirconia, YSZ(001), as a model substrate due to a nearly perfect lattice match. However, we found that for MBE growth of EuO/YSZ thermodynamics has to be considered as oxygen supply from YSZ causes the formation of Eu_2O_3 or Eu_3O_4. Based on an XPS study, we present a 4-step growth model of EuO/YSZ(001).

Moreover, we launchend the synthesis of EuO ultrathin films on pseudocubic $LaAlO_3$, LAO(001), which provides 4.2% tensile strain to EuO and is thus a candidate for tailoring a ferroelectric phase in EuO. We varied growth temperature and O_2 partial pressure in order to optimize the parameters for strained EuO/LAO and analyzed the resulting films using electron- and X-ray diffraction as well as magnetometry.

O 37.5 Tue 15:00 H16

Vanadium dioxide thin films on (100)- and (110)-oriented ruthenium dioxide islands — •Simon Fischer[1], Michael Foerster[2], Lucia Aballe[2], Vedran Vonk[3], Jens Falta[1], Jon-Olaf Krisponeit[1], and Jan Ingo Flege[4] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]ALBA Synchrotron Light Facility, Barcelona, Spain — [3]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [4]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus, Germany

Bulk vanadium dioxide exhibits a metal-insulator transition at 68 °C. Because this change in resistivity is linked to a structural transition, the transition temperature can be tuned by epitaxial strain. Due to the high lattice mismatch of RuO$_2$ with VO$_2$, this substrate promises a highly shifted transition temperature, which enables new types of switching devices, smart coatings, and sensors. It is prepared by oxidizing a Ru(0001) crystal, providing micron-sized, (110)- as well as (100)-oriented RuO$_2$ islands simultaneously.

One of the challenges in preparing VO$_2$ is to reliably meet the desired stoichiometry. We investigated the vanadium oxidation state using local XAS and XPS measurements taken at a synchrotron-based XPEEM instrument, revealing that VO$_2$ stoichiometry is maintained throughout the entire film. This was found not only on RuO$_2$(100) and RuO$_2$(110), but also on the bare ruthenium substrate. The VO$_2$ film thickness was determined to 3.6 nm by ex situ XRR measurements.

Financial support from the DFG is acknowledged.

O 37.6 Tue 15:15 H16

Ab-initio studies of the (110) surface terminations of rutile VO2 — •Jakub Planer, Florian Mittendorfer, and Josef Redinger — Vienna University of Technology, 1040 Vienna, Austria

Vanadium dioxide is a promising candidate for fast electronic or optical switching. These applications are based on a metal-insulator transition at 340 K, where the structure changes from a monoclinic to a rutile phase. Yet this transition is sensitive to the presence of strain or defects, such as oxygen vacancies. We present results for the bulk and surface properties of the VO2 phases under varying oxygen partial pressure, and compare our results to recent experimental findings. The calculations were performed with the Vienna Ab initio Simulation Package (VASP). We find that standard GGA functionals (PBE) offer an appropriate description of the structural properties of the rutile phase and monoclinic phase, but more advanced functionals such as meta-GGA approaches (SCAN) have to be employed to capture surface energies well. The stability of various surface terminations for the rutile (110) surfaces will be discussed in relation to experimental findings. For PBE we find a slightly oxidized tetrahedral termination under UHV conditions (μ = -1.88 eV). Using PBE+U (U = 2 eV) a buckled (110) termination is obtained from simulated annealing calculations. At last, we will present the results of an enlarged search for relevant surface terminations applying a state-of-the-art meta-GGA SCAN(+U) functional together with a first-principles genetic algorithm as implemented in the USPEX package.

O 37.7 Tue 15:30 H16

Surface reconstructions on VO$_2$(110) — •Jon-Olaf Krisponeit[1], Simon Fischer[1], Jan Ingo Flege[1,2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus, Germany

Vanadium dioxide features a pronounced metal-insulator transition at 340 K. For thin films, this transition is adjustable via substrate-induced strain, making VO$_2$ highly attractive for oxide electronic applications like switching devices and sensors. In addition, VO$_2$ is considered for smart coatings and as catalytic material. For such applicational efforts, a thorough understanding of the relevant surfaces is an important prerequisite.

Among the low-indexed surfaces orientations of VO$_2$, the (110) surface is energetically favorable. We have prepared VO$_2$(110) thin films by means of reactive molecular beam epitaxy on two different substrate types: TiO$_2$(110) single crystals as well as on RuO$_2$(110) islands grown on Ru(0001) crystals. The film stoichiometry was confirmed via XPS, while the surface structure was investigated by μLEED. For both substrate types diffraction patterns of three distinct symmetries have been observed in dependence on temperature. The corresponding surface reconstructions will be discussed in terms of surface oxygen content.

Financial support from the DFG and the Institutional Strategy of the University of Bremen, funded by the German Excellence Initiative, is acknowledged.

O 37.8 Tue 15:45 H16

Structural characteristics of oxide surfaces from quantum-mechanical calculations — •Maofeng Dou and Maria Fyta — Institute of Computational Physics, Universität Stuttgart,Allmandring 3, 70569 Stuttgart, Germany

Oxide surfaces are studied here by means of quantum-mechanical calculations implementing the density functional theory. We investigate different surfaces made of ZnO, TiO2, and SiO2. These are analyzed with respect to their structure and morphology. Through our simulations, we also assess their stability with respect to the different crystallographic planes taken to cut the surface from the bulk crystal. Amorphous surfaces are also considered and the influence of density and surface roughness is assessed. Our results underline the characteristics in their electronic properties, such as the electronic density of states and their band structure. These are compared to their bulk counterparts and show distinct features. In the end, we will discuss the relevance of these oxide surfaces in accommodating an organic layer to form inorganic/organic hybrid materials.

O 37.9 Tue 16:00 H16

Probing copper oxidation by in-situ optical spectroscopy — •Björn Maack and Niklas Nilius — Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany

The oxidation characteristic of metals stands in the focus of fundamental and applied research already for many decades. Standard rate-laws for oxidation, as predicted by Cabrera/Mott and Wagner, are typically valid only at the onset of oxide formation and deviate from the experimental findings with increasing oxide thickness. Using optical transmission spectroscopy, we have followed the process of copper oxidation in-situ at well-defined pressure and temperature conditions. The data were analyzed with the transfer-matrix method, including plasmonic, percolation and interference effects. The derived time-dependence of oxide growth reveals an accelerated rate at intermediate film thicknesses, in contrast to classical theories. This behavior is understood, if the increase of the reactive metal-oxide interface is considered together with the diffusive transport of the reactive species.

O 37.10 Tue 16:15 H16

Reduction and reoxidation of (111) and (100) oriented cerium oxide islands on Cu(111) — •Linus Pleines[1], Francesca Genuzio[2], Tevfik Onur Menteş[2], Andrea Locatelli[2], Jens Falta[1,3], and Jan Ingo Flege[4] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]ELLETRA Synchrotron Light Source, Basovizza, Italy — [3]MAPEX Center for Materials and Processes, Bremen, Germany — [4]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany

The conversion of CO$_2$ to methanol is an important process of high industrial potential. It could help solving the greenhouse gas problem (CO$_2$) and further provide methanol which can be used as a synthetic fuel. In order to lower the activation energy barrier of the reactions a catalyst is necessary. We studied the interaction of H$_2$ and CO$_2$ with ultrathin cerium oxide islands on a Cu(111) substrate observed by low-energy electron mircoscopy (LEEM), x-ray absorption spectroscopy (XAS) and resonant photoelectron spectroscopy (RPES). From earlier studies the orientation of the CeO$_x$ is known to be decisive for the catalytic activity. In our experiments CeO$_x$(100) is directly compared to CeO$_x$(111) via a side-by-side growth, so that the same conditions prevail during the experiment. At low temperatures no reduction of the CeO$_x$(111) and CeO$_x$(100) were observed. However, at a higher temperature the reduction was activated. Furthermore, we show that the exposure to CO$_2$ leads to the formation of partially reoxidized CeO$_x$ and saturation below CeO$_2$ with progressive CO$_2$ exposure.

O 37.11 Tue 16:30 H16

Evidence of a nanosize regime in oxide/metal heteroepitaxy — •Claudine Noguera[1], Jacek Goniakowski[1], Gregory Cabailh[1], Jacques Jupille[1], Rémi Lazzari[1], Jingfeng Li[1], Pierre Lagarde[2], and Nicolas Trcera[2] — [1]CNRS, Sorbonne Université, Institut des NanoSciences de Paris, UMR 7588, 4 Place Jussieu, F-75005 Paris, France — [2]Synchrotron SOLEIL, Orme des Merisiers, St-Aubin, BP48, F-91192 Gif sur Yvette, France

The growth mode of strained epitaxial films relies on the interaction strength, the lattice matching and the mechanical response of the system. The present work focuses on the basic physics of supported nano-islands by examining the characteristics of MgO/Ag(100) taken as a case study. By a combination of experiments and simulations, we highlight the existence of a small size regime in which, despite the largest adhesion and the smallest mismatch, the islands are the least distorted by the substrate. We assign this unexpected behaviour to the enhanced island stiffness which makes the cost of elastic distortion prohibitive compared to the associated gain of MgO-Ag interaction energy. The analysis provides a general framework to predict and/or understand nanoscale effects on interfacial pseudomorphy. These are likely to hold whatever the nature of the deposit and substrate under consideration. It may have far reaching consequences on many properties of supported nano-objects.

O 38: Organic Molecules on Inorganic Substrates II: Electronic Properties and Charge Transfer

Time: Tuesday 14:00–16:45 Location: H24

O 38.1 Tue 14:00 H24

Electronic properties of NiOEP on copper: a molecular orbital tomography study — •H. Sturmeit[1], G. Zamborlini[1], S. Ponzoni[1], M. Jugovac[2], V. Feyer[2], C. M. Schneider[2], and M. Cinchetti[1] — [1]TU Dortmund, 44227 Dortmund, Germany — [2]Forschungszentrum Jülich, 52428 Jülich, Germany

π-conjugated organic molecules are considered a valuable alternative to inorganic semiconductors as their electronic, optical and magnetic properties can be tailored at the atomic level. Supporting organic films with metal substrates within an organic-based device, may lead to chemical reactions, hybridization, and/or charge transfer at the metal/organic interface, ultimately affecting the device performance. Recently, this has been shown for nickel tetraphenylporphyrin (NiTPP) evaporated on Cu(100), whose frontier orbitals get partially filled up to the LUMO+3 [Zamborlini et al, Nat. Comm. 8, 335, 2017] due to a consistent charge transfer at the interface. In the present work, we studied the impact of the peripheral substituents of the porphyrin macrocycle on the charge transfer. To achieve this goal, nickel octaethylporphyrin (NiOEP) molecules, where the four phenyl ligands are replaced with eight ethyl terminations in the β-positions of the pyrrole moieties, were sublimated on the (100) copper surface. The overall energy level alignment at the metal/organic interface was characterized by means of molecular orbital tomography. Our preliminary measurements show that changing the periphery does not strongly influence the overall charge transfer: the LUMO+3 remains partially filled while shifting its energetic position by a few tens of meVs.

O 38.2 Tue 14:15 H24

Molecular Orbital Imaging Beyond the First Monolayer — •Christian Metzger[1], Manuel Grimm[1], Martin Graus[1], Kiana Baumgärtner[1], Matteo Jugovac[2], Giovanni Zamborlini[2], Vitaliy Feyer[2], Achim Schöll[1], and Friedrich Reinert[1] — [1]Julius-Maximilians-Universität Würzburg, Experimental Physics VII, 97074 Würzburg, Germany — [2]Forschungszentrum Jülich GmbH, Paul Grünberg Institute (PGI-6), 52425 Jülich, Germany

We present a method to determine the geometric alignment of molecular compounds within evaporated thin films by a combination of experimental orbital imaging combined with photoemission matrix element calculations on the example of pentacene bilayers on Ag(110). The technique utilizes angle-resolved photoemission spectroscopy (ARPES) measurements at a photoemission electron microscope in Fourier-space imaging mode (kPEEM), which enables the efficient detection of photoelectrons emitted into the entire hemisphere above the sample. By simulating different tilt angles of isolated pentacene molecules and comparing the resulting photoemission intensity distribution with momentum maps measured on molecular multilayers, one is able to determine the molecules' tilt angles for each separate layer independently from one another. We determine that the flat-lying molecules of the first monolayer on the metal substrate exhibit a noticable tilt angle upon adsorption of a second molecular layer. The molecules in the second layer above the substrate feature a larger inclination, which is evidence of the gradual relaxation into the pentacene bulk structure with increasing film thickness.

O 38.3 Tue 14:30 H24

Strong and weak interactions of metal organic networks with metal surface: adsorption geometry and electronic structure. — •Iulia Cojocariu[1], Matteo Jugovac[1], Giovanni Zamborlini[2], Vitaliy Feyer[1], and Claus M. Schneider[2,3] — [1]PGI-6, Forschungszentrum Jülich GmbH, Germany — [2]TU Dortmund, Exp. Phys. VI, Germany — [3]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Germany

We report a study of the adsorption behaviour of iron phthalocyanine (FePC) in the first and second layer atop of low-index crystal faces of silver. The combination of low-energy electron diffraction and molecular orbital tomography (MOT) allows the determination of the superstructure unit cell and the azimuthal orientation of the molecules with respect to the substrate. Additionally, momentum patterns give information about the electronic structure and the symmetry of molecular orbitals in the first and second organic layer.

Within the MOT approach, it is possible to disentangle the contribution of the first and the second FePC long-range ordered layers to the whole valence band spectrum. While the first exhibit strong hybridization and charge transfer with the metal surface (as pointed by partially filled LUMOs in the momentum maps), the second is decoupled. This analysis allows us to understand the peculiarities of the phenomena at the organic/metal interface.

Experiments were carried out at the NanoESCA beamline at Elettra. The setup includes a PEEM that directly images parallel momentum component (k_x,k_y) of emitted photoelectrons at a fixed binding energy.

O 38.4 Tue 14:45 H24

Spin- and angle-resolved photoemission study of heteromolecular bilayer films on ferromagnets — •Benito Arnoldi[1], Stefan Lach[1], Robert Ranecki[1], Johannes Stöckl[1], Mirko Cinchetti[2], Benjamin Stadtmüller[1], Christiane Ziegler[1], and Martin Aeschlimann[1] — [1]Department of Physics, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]Experimentelle Physik VI, Technische Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

Heteromolecular bilayer films on ferromagnetic surfaces are highly intriguing molecular assembles to study and control the spin-dependent electronic properties of these so called spinterfaces. In these systems, the first molecular layer is strongly hybridized with the surface while the molecular character of the second layer molecules is largely preserved.

Here, we focus on such a heteromolecular bilayer film consisting of C60 grown on the CuPc/Co(001) interface. The spin dependent electronic structure of this adsorbate system is investigated by spin- and angle resolved photoemission. Using a dedicated data analysis scheme, we are able to distinguish the formation of hybrid interface states at the CuPc/Co interface as well as charge transfer induced interface states at the heteromolecular interfaces from elastic scattering effects of photoelectrons in the molecular stack. Our results will be discussed in the light of local scanning tunnel spectroscopy data recorded for the same material system. This allows a direct assignment of spectroscopic signals to the different parts of the heteromolecular bilayer film.

O 38.5 Tue 15:00 H24

Electronic decoupling of PTCDA by a single layer of hexagonal boron nitride on Cu(111) — •Christine Brülke[1], Timo Heepenstrick[1], Ina Krieger[1], Beatrice Wolff[1], Xiaosheng Yang[2], Ali Shamsaddinlou[2], Simon Weiss[2], Francois C. Bocquet[2], F. Stefan Tautz[2], Serguei Soubatch[2], and Moritz Sokolowski[1] — [1]Universität Bonn, Institut für Physikalische und Theoretische Chemie, 53115 Bonn, Germany — [2]Forschungszentrum Jülich, Peter Grünberg Institut (PGI-3), 52425 Jülich, Germany

Hexagonal boron nitride (hBN) has previously been investigated regarding its function as a template for organic molecules as well as its ability to decouple them from an underlying metal substrate. We report on the ability of hBN to decouple the model molecule PTCDA from a Cu(111) substrate using structural and spectroscopic methods and present quantitative data that characterize the adsorption complex. SPA-LEED and STM investigations show that the lateral structure of the monolayer conforms to the (102) planes of the bulk configurations within less than 4%. NIXSW experiments reveal that the molecules are positioned at a large distance of 3.38 Å above the surface with a very small distortion out of the molecular plane by only 2.6%. Furthermore, photoelectron spectroscopy (XPS, UPS) shows that there is no hybridization of molecular and metal states. All of these features differ significantly from those found for PTCDA on metal surfaces. The electronic decoupling of the PTCDA molecule from the metal substrate is further proven by the non-vanishing fluorescence yield of the monolayer because otherwise mixing of electronic states leads to quenching.

O 38.6 Tue 15:15 H24

Using self-assembled monolayers for controlling charge-carrier injection into organic transistors — Andreas Petritz[1], Markus Krammer[2], Eric Sauter[3], Michael Gärtner[4], Giulia Nascimbeni[2], Andreea Cojocaru[1], Esther Karner-Petritz[1], Roland Resel[2], Andreas Terfort[4], Michael Zharnikov[3], Karin Zojer[2], Barbara Stadlober[1], and •Egbert Zojer[2] — [1]Joanneum Research, MATERIALS-Institute for Surface Technologies and Photonics, Austria — [2]Institute of Solid State Physics, Graz University of Technology, Austria — [3]Applied Physical Chemistry, Heidelberg University, Germany — [4]Institut für Anorganische und Analytische Chemie, Goethe-University Frankfurt, Germany

We show how self-assembled monolayers (SAMs) bearing embedded polar groups can be used for tuning contact resistances in organic thin-film transistors by three orders of magnitude.[1] The chosen approach also allows the realization of flexible p- and n-type transistors using Au electrodes.[1] An in-depth surface science investigation of the SAMs and the organic layers grown on top of them [1,2,3] show that the tunability of the contact resistance is a consequence of SAM-induced work function changes. Additionally, the dependence of tunneling transport through the SAMs on their chemical structure plays an important role.[1,4] The experimental results are rationalized by density-functional theory calculations. [1] A. Petritz et al., Adv. Funct. Mater., 1804462 (2018). [2] M. Gärtner et al., J. Phys. Chem. C, published on-line [3] T. Abu-Husein et al., Adv. Funct. Mater. 25, 3943 (2015). [4] A. Kovalchuk et al., Chem. Sci. 7, 781 (2016)

O 38.7 Tue 15:30 H24

Reliable Modeling of the Charge Transfer Mechanism at Inorganic/Organic Interfaces — •Elisabeth Wruss, Egbert Zojer, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Graz, Austria

Charge transfer between substrate and adsorbate is one of the determining factors for the electronic structure at inorganic/organic interfaces. In this work we raise the question how well this property can be simulated using DFT and how the results are influenced by the chosen methodology as well as by assumptions regarding the interface structure. We focus on hybrid functionals, elucidating the interplay between the charge transfer mechanism (integer vs. fractional charge transfer) and the applied amount of Hartee-Fock-like exchange. As an exemplary system, we use tetrafluoro-1,4-benzoquinone adsorbed on Cu and Cu2O. We find that the simulated charge transfer mechanism is determined by a delicate interplay of the DFT functional and the physical properties of the system, such as hybridization strength, the size of the adsorbed molecule, and the surface polarizability. As a next step, we go beyond the simplified idea of perfect metallic or insulating substrates and include surface defects. By acting as reaction centers, such defects strongly impact the interaction between substrate and adsorbate and lead to charge transfer even in situations in which this would not be expected for idealized systems. Our results highlight that not only a proper choice of the DFT functional, but also the consideration of realistic, defect-afflicted surfaces is crucial for reliably modeling charge transfer at interfaces.

O 38.8 Tue 15:45 H24

Modifying the tunneling decay coefficients of self-assembled monolayer junctions — Xiaoping Chen[1], Harshini Annadata[1], •Bernhard Kretz[2], David Alexander Egger[2], and Christian Nijhuis[1,3,4] — [1]Department of Chemistry, National University of Singapore, Singapore — [2]Institute of Theoretical Physics, University of Regensburg, Regensburg, Germany — [3]Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, Singapore — [4]NUSNNI-Nanocore, National University of Singapore, Singapore

The development and improvement of molecular electronic devices requires insight into charge transport across organic-inorganic interfaces. Charge transfer rates in the quantum tunneling transport regime strongly depend on the tunneling decay coefficient β, which determines the decline of the current across the junction as a function of the length and the barrier height. It is well-known that the value of β of self-assembled monolayer (SAM) junctions depends on the specific electronic structure of the molecular backbone. Combining experiments and computer simulations, we demonstrate that β of a non-conjugated SAM junction can be altered by using different halogens as termination on one side of the molecular backbone. Our experiments indicate that this modification of the tunneling coefficient is correlated with a change in the dielectric constant. Furthermore, our calculations shed some light on how the frontier orbitals and transmission channels are affected by the change of the end-group.

O 38.9 Tue 16:00 H24

Charge distribution within molecular dipoles and their influence on the local work function of the substrate — •Sergey Trishin[1], Daniela Rolf[1], Christian Lotze[1], Philipp Rietsch[2], Siegfried Eigler[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institut für Chemie und Biochemie, Freie Universität Berlin, 14195 Berlin, Germany

Donor-acceptor (DA) molecules exhibit two charge-separated moieties, which makes them interesting for application in molecular electronics. However, deposition on metal surfaces, which may be necessary for certain applications, can alter the charge distribution of DA molecules due to screening and hybridization effects.

We study Ethyl-Diaminodicyanoquinone molecules on a Au(111) surface with scanning tunnelling microscopy (STM) and non-contact atomic force microscopy (nc-AFM). By mapping the local contact potential difference (LCPD) over the molecules we show that the intrinsic dipole moment of the molecules is partially preserved upon adsorption on the Au(111) surface. Moreover the molecular orbitals appear to be shifting across the molecule. This shift follows the variation of the LCPD signal. Both findings can be explained by vacuum-pinned energy levels and local changes in the work function due to the molecular charges. An overall reduction of the work function is related to a local scale push-back effect. There molecules push back substrate electrons, which are leaking out into the vacuum.

O 38.10 Tue 16:15 H24

Mixed monomolecular films with embedded dipolar groups on Ag(111) — Eric Sauter[1], Charles-Olivier Gilbert[2], Jean-François Morin[2], Andreas Terfort[3], and •Michael Zharnikov[1] — [1]Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [2]Département de Chimie and Centre de Recherche sur les Matériaux Avancés,Université Laval, Québec, Canada G1V 0A6 — [3]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, 60438 Frankfurt, Germany

We studied the application of the concept of embedded dipole in monomolecular self-assembly to the Ag(111) substrate, using two different types of molecules with either pyrimidine groups embedded into aromatic backbones or ester groups embedded into aliphatic backbones as test systems. The orientation of the embedded group was varied and the molecules with the oppositely oriented dipoles were combined together as mixed self-assembled monolayers (SAMs). Pronounced electrostatic effects of the dipolar groups were observed, reflected, in a consistent manner, by the electrostatic shift in photoemission and by work function variation. The character and extent of these effects could be explained in context of molecular orientation. The pyrimidine-substituted SAMs were found to be especially useful for the electrostatic interface engineering, allowing, in the case of Ag, a flexible tuning of the work function in the ca. 0.85 eV range without changing the character of the SAM-substrate and SAM-ambient interfaces. An analogous behavior can also be expected for other substrates.

O 38.11 Tue 16:30 H24

Understanding the interplay of chemical and electrostatic effects for the core level spectra characterizing metal-organic interfaces — •Giulia Nascimbeni[1], Michael Zharnikov[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Applied Physical Chemistry, Heidelberg University, Germany

Polar organic monolayers (POMs) are widely used in the field of organic electronics to manipulate the work function of metallic electrodes. This results from the ordered assembly of polar units giving rise to collective electrostatic effects. Interestingly, the latter have also been shown to impact the core level energies of the POMs [1]. Consequently, these effects, reflected as electrostatic shifts, can be conveniently monitored by X-ray photoelectron spectroscopy (XPS) [2-4]. For core-level excitations from atoms close to the substrate, the situation becomes more involved, as adsorption-induced charge rearrangements can also give rise to chemical shifts. In this contribution we present density functional theory (DFT) calculations for such cases. They allow a reliable interpretation of XPS data by addressing the interplay of chemical and electrostatic shifts. Our analysis highlights how the combination of DFT and XPS works as a powerful tool for the investigation of electronic and also structural properties of interfaces. [1] Taucher et al., J. Phys. Chem. C, 2016, 120, 3428. [2] Sauter et al., J. Phys. Chem. C, 2018, 122, 19514. [3] Hehn et al., J. Phys. Chem. Lett., 2016, 7, 2994. [4] Cabarcos et al., J. Phys. Chem. C, 2017, 121, 15815.

O 39: Poster Tuesday: 2D Materials

Time: Tuesday 18:00–20:00 Location: Poster D

O 39.1 Tue 18:00 Poster D

Electric pathways on the nanoscale — •Johannes Aprojanz[1], Pantelis Bampoulis[2,4], Alexei A. Zakharov[3], Harold J. W. Zandvliet[2], and Christoph Tegenkamp[1,4] — [1]Institut für Physik, Technische Universität Chemnitz, Germany — [2]Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — [3]MAX IV Laboratory and Lund University, 221 00 Lund, Sweden — [4]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

The electronic performance of graphene nanoribbons (GNRs) is essentially influenced by their edge termination and environment. Hence, the integration of these graphene nanostructures in future carbon-based nanoelectronics demands a profound understanding of charge transport as well as the identification of defects and interactions with the substrate, which crucially limit the propagation of charge carriers. In this study, we explore the electronic properties of both zig-zag (zz) and armchair (ac) GNR epitaxially grown on SiC templates. By means of comprehensive lateral force, conductive atomic force and nanoprobe measurements, we have directly imaged a nanoscale conductive channel, located at the bottom edge of a zz-GNR, and confirmed its ballistic nature by probe spacing dependent nanoprobe measurements. SiC substrate steps were identified as dominant charge scattering centers for this edge mode. Semi-conducting characteristics were observed for ac-GNR caused by the nano-faceting of the sidewall resulting in an array of mini-terraces. Finally, we have assigned buffer layer formation on flat SiC nanoterraces and suspended GNRs at their step edges.

O 39.2 Tue 18:00 Poster D

Intricacies in Twisted bilayer graphene: Structural or Electronic? — •Birce Sena Tömekce[1], Büsra Gamze Arslan[1], Oguzhan Gürlü[1,2], and Dilek Yildiz[1,2] — [1]Istanbul Technical University, Department of Physics, 34460, Istanbul, Turkey — [2]Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland

Electronic and morphological properties of twisted bilayer graphene strongly depend on the rotation angle between the layers. Super periodic structures called as moire patterns are formed as a result of such rotation. However, properties of single/bilayer graphene may be modified due to unintentional doping by the substrate or due to the stress that is induced by lattice mismatch between graphene and the substrate. We prepared moire structures on highly oriented pyrolytic graphite (HOPG) by rotating the topmost graphene layer. This way we avoid the effect of the substrate on the final bilayer as the graphene is on its native surface. We studied the electronic and morphological properties of different moire patterns on graphene/HOPG system by means of scanning tunneling microscopy (STM) and spectroscopy (STS). We studied apparent corrugations of different moire patterns as a function of bias voltage in order to compare the electronic properties of moire patterns as a function of their periodicities [1]. In this work we discuss the formation mechanism of moire patterns in HOPG surfaces. We also show that moire patterns are mostly electronic if the rotation angle of the topmost graphene layer is relatively large and they are structural if the rotation angle is comparatively small. [1] D. Yildiz and O. Gürlü, Mater. Today Commun., 8 (2016), pp. 72-78

O 39.3 Tue 18:00 Poster D

Transport Experiments Through Individual Graphene Nanoribbons — •Niklas Friedrich[1], Jingcheng Li[1], Pedro Brandimarte[2], and Nacho Pascual[1,3] — [1]CIC nanoGUNE, 20018 San Sebastian-Donostia (Spain) — [2]Donostia International Physics Center, 20018 San Sebastian-Donostia (Spain) — [3]Ikerbasque, Basque Foundation for Science, 48013 Bilbao (Spain)

The bottom-up synthesis of atomically precise graphene nanoribbons (GNRs) envisions the production of model graphene structures with tuned electrical properties for electronic transport. However it is difficult to access experimentally the unperturbed bandstructure of ribbons, and furthermore, to probe their behaviour as electron transporting bands. In most scanning tunnelling spectroscopy (STS) experiments the GNRs are absorbed on a metallic substrate. This leads to a hybridization of the electronic orbitals of the GNRs with the metal and consequently a perturbation of the bandstructure.

Here we use the STM tip to contact one termination of 7-armchair GNRs with different functionalizations and partially lift them from the surface, to bridge tip and sample in a typical transport configuration. Such, the hybridization between GNR and substrate is reduced and we probe the effect on the GNR's band strucuture as transport channels. We study the evolution of the bandstructure during the lifting process for varying functionalization and compare our experimental results to DFT calculations.

O 39.4 Tue 18:00 Poster D

Chemical stability of graphene nanoribbons exposed to ambient conditions — •Mohammed S. G. Mohammed[1,2], James Lawrence[1,2], Alejandro Berdonces Layunta[1,2], Luciano Colazzo[1,2], Diego Peña[3], and Dimas G. de Oteyza[1,2,4] — [1]Donostia International Physics Center (DIPC), San Sebastian, Spain — [2]Materials Physics Center, Centro de Física de Materiales (CSIC/UPV-EHU), San Sebastian, Spain — [3]Centro de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS), Departamento de Química Orgánica, Universidade de Santiago de Compostela, Santiago de Compostela, Spain — [4]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Graphene nanoribbons (GNRs) are extremely promising materials for optoelectronic applications. Key for the potential use of these functional materials synthesized under ultra-high vacuum is their stability to the environments faced during the device implementation, as well as during the ultimate device operation. In this work, starting from atomically precise chiral GNRs with well-defined semiconducting properties, we study the effect of their exposure to atmospheric conditions. STM high-resolution images and spectroscopic analysis show the severe degradation of both the bonding structure and the associated electronic properties of the ribbons. Through control experiments exposing the GNRs, still under vacuum, to low partial pressures of pure oxygen, we reveal its key role in the GNRs degradation.

O 39.5 Tue 18:00 Poster D

Moiré structure of MoS_2 on Au(111): Local structural and electronic properties — Nils Krane, •Christian Lotze, and Katharina J. Franke — Freie Universtät Berlin, Berlin, Germany

Single-layer molybdenum disulfide (MoS_2) has been of large interest in the latest years, due to features like a direct band gap, a strong spin-splitting of the valence band at the K-point or as a decoupling layer for molecules in an STM junction [1].

Here we grow MoS_2 epitaxially on a Au(111) surface and investigate its local structural and electronic properties. Using a combined STM/AFM at low temperatures we can identify the two different hollow sites in the Moiré superstructure and thus the orientations of the MoS_2 islands. Consequently we find a unique stacking order of MoS_2 with respect to the first two layers of the Au(111) surface [2].

Furthermore we get an insight into the band structure of MoS_2 with an STM [3] by measuring the decay length κ of the tunneling current, which depends on $k_{\|}$. We find a strong spatial dependence of κ, which we ascribe to the Moiré reconstruction of MoS_2 on Au(111). Additionally we find 0.4 eV above the conduction band minimum an MoS_2 state at the Γ point. We ascribe its existence to the interaction between the Au(111) substrate and the MoS$_2$.

[1] Krane, *et al.*, ACS Nano, 2018, 12, 11, 11698-11703
[2] Krane, *et al.*, Surface Science, 2018, 678, 136-142
[3] Zhang, *et al.*, Nano Lett., 2015, 15, 10, 6494-6500

O 39.6 Tue 18:00 Poster D

h-BCN Monolayers - a graphenic two-dimensional semiconductor — •Christoph Dobner[1], James Hooper[2], Sumit Beniwal[3], Daniel P Miller[4], Shi Cao[5], Peter A Dowben[5], Eva Zurek[4], and Axel Enders[1,5] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth — [2]Dept. of Theoretical Chemistry, Jagellionian University, 30-060 Krakow, Poland — [3]Universität Erlangen-Nürnberg, 91058 Erlangen — [4]Dept. of Chemistry, Buffalo, New York 14260, USA — [5]Dept. of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588, USA

The structural and electronic properties of a 2D graphenic but ternary monolayer containing atoms of carbon, nitrogen, and boron, *h*-BCN, is discussed based on results from scanning tunneling microscopy, angle-resolved photoelectron spectroscopy and first-principles calculations. The epitaxial relationship between film and the Rh(111) substrate is manifested in a Moiré pattern in LEED and in the periodic buckling of the film on the substrate itself. The band structure and notably the band gap is consistent with that of a semiconductor and of the order of 2 - 3 eV. The valence band structure of *h*-BCN is dominated by bands formed of highly delocalized electrons, with an effective hole mass of $-0.2\mathrm{m}_e$. The lowest-energy structural model obtained for a 2D structure wherein the precursor molecules do not thermally decompose during film growth reproduces key features of the band structure, most notably a direct semi-conducting band gap at the K-point. However, other potential *h*-BCN model structures that break the connectivity of the precursor molecule can be imagined and will be discussed.

O 39.7 Tue 18:00 Poster D

Study of the morphology and the Dirac-type band structure of 2D semi-conductor superlattices with honeycomb geometry — •Pierre Capiod, Tomas Meerwijk, Joep Peters, Christiaan Post, and Daniel Vanmaekelbergh — Condensed Matter and Interfaces, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, Netherlands

2D systems with honeycomb geometry have attracted considerable interest in the last decade with unique electronic properties. Among them, the band structure of those type of materials exhibits a Dirac cone close the K-point. It would be of high interest to combine both Dirac-type band structure with the inherent semiconductor properties such as band gaps for electrical or optical switching.

The self-assembly of PbSe and CdSe semiconductor nanocrystal is possible via state-of-the-art chemistry techniques resulting in the square geometry or the wanted honeycomb geometry. Tight-binding calculations on the honeycomb geometry with CdSe nanocrystals have shown clear Dirac cones in the conduction bands and an opened Dirac cone in the valence band. The band structure exhibits as well non-trivial flat bands due to interactions between P-type orbitals.

The poster will show the results on the morphology and the characterization of the electronic properties obtained via Scanning Probe Microscopy (AFM & STM/STS). It will describe the steps from the synthesis, the preparation of the samples in UHV via annealing and ion bombardment to the characterization via LT-STM.

O 39.8 Tue 18:00 Poster D

Luttinger liquid in a box: spectral signature of spin-charge separation in MoS$_2$ mirror twin boundaries — •Philipp Weiss[1], Wouter Jolie[2,3], Clifford Murray[2], Joshua Hall[2], Fabian Portner[1], Nicolae Atodiresei[4], Arkady Krasheninnikov[5,6], Carsten Busse[2,3,7], Hannu-Pekka Komsa[6], Thomas Michely[2], and Achim Rosch[1] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]II. Physikalisches Institut, University of Cologne, Germany — [3]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [4]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [5]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [6]Department of Applied Physics, Aalto University, Finland — [7]Department Physik, Universität Siegen, Germany

Electrons in one dimension are expected to fractionalize into spin and charge degrees of freedom. A candidate for the realization of a one-dimensional electron system are mirror twin boundaries in MoS$_2$. Scanning tunneling spectroscopy indicates the doubling of states, well separated in energy due to the finite length of the boundaries.

To uncover the nature of these states we calculate the local density of states of interacting electrons in a box, using Tomonaga-Luttinger liquid theory. Comparison with the experimental spectra allows us to identify the doubled states as emergent spin and charge excitations.

O 39.9 Tue 18:00 Poster D

Ab initio study of light-switchable properties of azobenzene-functionalized MoS$_2$ — •Helena Osthues and Nikos Doltsinis — Institute of Solid State Theory, Westfälische Wilhelms-Universität, 48149 Münster, Germany

The optical and electronic properties of multilayer molybdenum disulfide and other transition metal dichalcogenides (TMDCs) crucially depend on the interlayer spacing and, in general, on the surrounding dielectric medium [1]. We investigate layered two-dimensional materials which can reversibly alter their properties by exploiting the photoinduced *E-Z* isomerisation of covalently attached azobenzene chromophores.

In the present study, the stability of different functionalizations is analysed, and the photoswitching mechanism is studied using excited state ab initio molecular dynamics based on time-dependent density functional theory (TDDFT). The band structure and the absorption spectrum of the 2D structures are treated within the many-body perturbation theory in the *GW* approximation using a perturbative LDA+GdW approach [2] to take into account the variations in polarization and dielectric screening.
[1] Splendiani, A. *Nano Lett.* 2010, *10*, 1271.
[2] Rohlfing, M. *Phys. Rev. B* 2010, *82*, 205127.

O 39.10 Tue 18:00 Poster D

Preparation of Graphene Bilayers on Platinum by Sequential Chemical Vapor Deposition — Johannes Halle, •Alexander Mehler, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, Ilmenau, Germany

A cheap and flexible method is introduced that enables the epitaxial growth of bilayer graphene on Pt(111) by sequential chemical vapor deposition. Extended regions of two stacked graphene sheets are obtained by, first, the thermal decomposition of ethylene and the subsequent formation of graphene. In the second step, a sufficiently thick Pt film buries the first graphene layer and acts as a platform for the fabrication of the second graphene layer in the third step. A final annealing process then leads to the diffusion of the first graphene sheet to the surface until the bilayer stacking with the second sheet is accomplished. Scanning tunneling microscopy unravels the successful growth of bilayer graphene and elucidates the origin of moiré patterns.

O 39.11 Tue 18:00 Poster D

Non-contact Energy Dissipation Through Charge Density Waves on 1T-TaS2 — •Dilek Yildiz, Marcin Kisiel, Urs Gysin, and Ernst Meyer — University of Basel, Department of Physics, Basel, Switzerland

Small amount of energy is dissipated when bodies separated by a few nanometers gap are in relative motion. Non-contact friction can be measured by a highly sensitive cantilever oscillating like a tiny pendulum over the surface. This phenomena have been studied in many systems revealing structural and electronic phase transitions, quantum dots, and graphene devices. Understanding the origin of various dissipation mechanisms is still a wide open problem. Such frictional nature of layered systems, such as charge density wave (CDW) systems awaits to be investigated. Different phases of CDW on 1T-TaS2, a layered transition metal dichalcogenide (TMD), can be observed at different temperatures. The phase transition between nearly-commensurate and commensurate phases occurs at 180 K. We studied the origin of non-contact energy dissipation mechanisms on nearly-commensurate and commensurate CDW on 1T-TaS2. We studied the effect of Mott insulating state on dissipated power. The low temperature experimental results indicate that the main dissipation mechanism is Joule dissipation on commensurate CDW phase and fluctuation driven dissipation is the main mechanism on nearly-commensurate CDW phase. The spectroscopy performed on nearly commensurate phase of CDW indicates that the source of the fluctuating force and dissipation is the collective movement of weakly pinned charge density waves at room temperature.

O 40: Poster Tuesday: Adsorption and Catalysis

Time: Tuesday 18:00–20:00 Location: Poster D

O 40.1 Tue 18:00 Poster D

Wetting Properties of Electrochemically Active Polycrystalline CuFeO2, CuMO2 and CuFexM1-xO2 Delafossite Porous Surfaces — Robert A. Wheatley, Martin Roble, Sebastian Molina, •Diego Diaz, Susana D. Rojas, Birger Seifert, Sascha Wallentowitz, Donovan E. Diaz-Droguett, and Ulrich G. Volkmann — Institute of Physics and CIEN-UC, Pontificia Universidad Catolica de Chile, Av. Vicuna Mackenna 4860, Santiago, Chile

Delafossite type ternary oxides are considered favorable catalytic/photo-catalytic materials for a range of chemical reactions. For water-based reactions, hydroxylization, a process connected to the wettability of the surface, can greatly influence catalytic activity of a metal oxide. We investigate the wetting properties of CuFeO2, CuAlO2, CuGaO2 and composite CuFexM1-xO2 Delafossite oxides synthesized using hydrothermal and solid state methods. The materials display significant variance in wetting properties, from highly hydrophobic CuFeO2 as-grown powder, to complete wetting for porous cold-pressed pellets. After annealing treatments at relatively low temperatures $T > 300$ degree C the surfaces displayed permanent superhydrophilicity and a rapid absorption of H2O droplets via intergranular porosity. Acknowledgements: CONICYT Fellowship (MR) and Anillo CONICYT-PIA ACT 1409.

O 40.2 Tue 18:00 Poster D

Adsorption of Hydrogen Atoms on Aluminiumoxide — •Martin Liebetrau and Jörg Behler — Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany

The adsorption of atomic hydrogen is important in many fields, from heterogeneous catalysis and hydrogen storage to interstellar hydrogen on dust grains and nuclear fusion. Here, we report molecular dynamics simulations of high-energy hydrogen atom scattering at α-Al_2O_3. Employing a high-dimensional neural network potential, which allows us to include the full-dimensional thermal motion of the surface atoms, we are able to calculate a large number of trajectories with the accuracy of density-functional theory. Probing different kinetic energies and incident angles, we are able to characterize the interaction with the surface in detail.

O 40.3 Tue 18:00 Poster D

Water splitting reactions at clean and water adsorbed lithium niobate surfaces — •Christof Dues[1], Wolf Gero Schmidt[2], and Simone Sanna[1] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Department Physik, Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

Ferroelectric lithium niobate is a promising substrate for catalytic reactions. Yet, water splitting reactions aiming at hydrogen production are difficult to establish. Employing DFT and a simplified thermodynamic approach to calculate Gibbs energy differences, we present an efficient method to estimate the over-potentials related to the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) on both pristine $LiNbO_3(001)$ surfaces [1]. Our calculations show that the OER and HER over-potentials are lower on the negative (1.27 V) and positive (0.39 V) surface, respectively. The aqueous environment, simulated by water fragments adsorbed to the surface, changes the tendencies of the reactions: The OER over-potential becomes lower on the positive surface (1.07 V), and the HER over-potential at the negative surface (1.2 V).

[1] C. Dues, W. G. Schmidt and S. Sanna, *Water Splitting Reaction at Polar Lithium Niobate Surfaces*, submitted (2018).

O 40.4 Tue 18:00 Poster D

Amorphous oxide surfaces and their reactivity towards water dissociation — •Hannah Schlott and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Surface science studies on oxides mostly focus on the physical and chemical properties of single-crystal terminations. In nature, however, oxides are often amorphous and covered by hydroxyl groups and residual water. By using Car-Parrinello Molecular Dynamics (CPMD) and a melt-quench procedure we have created a series of realistic amorphous oxide surface structures. A new technique has been applied which allows a direct preparation of amorphous surfaces without requiring a retrospective cleavage of the amorphous bulk. Simultaneously, other species, such as hydroxyl groups, can be incorporated seamlessly into the amorphous surfaces. The reliability of the method is demonstrated for the oxides ZnO, TiO_2 and Al_2O_3. In a next step we analyzed the reactivity of the amorphous oxide surfaces towards water dissociation. For the example of amorphous ZnO we discuss typical water adsorption features and binding modes. Furthermore, we describe proton hopping events and chains of proton transfer reactions at the water/oxide interface.

O 40.5 Tue 18:00 Poster D

Structure evolution of oxide-supported Pt nanoparticles under reaction conditions — •Junjun Wang, Alexei Nefedov, Christof Wöll, and Yuemin Wang — Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Noble metal nanoparticles (e.g. Pt) dispersed on oxide supports have attracted great interest due to their high catalytic activity for various chemical reactions. Despite extensive investigations, a thorough understanding of the structure-activity relationship remains still a major challenge. In this work, the structure evolution of oxide-supported Pt nanoparticles (NPs) under different conditions was monitored by temperature-dependent infrared (IR) spectroscopy using CO as a probe molecule in combination with grazing-emission XPS. For Pt/CeO_2 it was found that Pt NPs vary substantially in size and oxidation state depending on the reductive/oxidative conditions. The IR data together with high-resolution TEM results obtained for Pt/Al_2O_3 catalysts revealed the presence of Pt particles/clusters with different shape and size ranging from isolated atoms to sub-nanometer clusters and ordered NPs. Our results allowed to gain deep insight into the structure evolution of various Pt species during the course of propane dehydrogenation reaction.

O 40.6 Tue 18:00 Poster D

Lattice formation and binding of metal clusters to hexagonal boron nitride on Ir(111) — •Moritz Will[1], Nicolae Atodiresei[2], Vasile Caciuc[2], Tobias Hartl[1], Pantelis Bampoulis[1], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Peter Grünberg Institut (PGI) and Institute for Advanced Simulation (IAS), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Moirés of two-dimensional materials on metal single crystal surfaces have a templating effect upon metal deposition from the gas phase, which can result in the formation of cluster superlattices. In particular, the moiré of hexagonal boron nitride (h-BN) on Ir(111) has been recently found to template Ir clusters into highly regular arrays with a thermal stability against sintering which far exceeds all other known substrates. [1]

Here we analyze the universality of the templating effect of h-BN/Ir(111) and compare the properties of other metal cluster arrangements to Ir clusters on h-BN/Ir(111). Scanning tunneling microscopy reveals cluster lattices of Pt can be grown with a number density per unit cell of $n = 1$ at room temperature. Au cluster lattices reach $n = 0.7$ for room temperature deposition, while for the case of Fe, deposition at 40 K enables superlattice formation with $n = 0.7$, stable at 300 K. Moreover, we analyze in detail for the case of Ir clusters the binding mechanism through selective hybridization of B and N atoms with the underlying substrate.

[1] Will, M., et al., ACS Nano (2018)

O 40.7 Tue 18:00 Poster D

A microscopy approach to investigating the energetics of small supported metal clusters — Barbara A J Lechner, Fabian Knoller, Alexander Bourgund, •Sebastian Kaiser, Ueli Heiz, and Friedrich Esch — Department of Chemistry & Catalysis Research Center, Technical University of Munich, Lichtenbergstr. 4, D-85748 Garching

We present examples of cluster dynamics observed via fast scanning tunneling microscopy (FastSTM). To that purpose, we have boosted the temporal resolution of our commercial STM up to 16 frames per second with a specially developed add-on electronics module [1], allowing us to match the frame rate to surface dynamics observed at elevated temperatures. On the example of small Pd clusters supported on a hexagonal boron nitride nanomesh on Rh(111), we observed a range of different dynamics [2]. Cluster diffusion within a nanomesh pore changes with adsorbate size: While atoms diffuse along the rim of the pore, a small cluster experiences a corrugation in the potential energy landscape and jumps between six sites around the pore center. The difference can be explained by the additional internal degrees of freedoms of a cluster. Furthermore, we monitored the reversible switching between two structural isomers of Pd clusters in situ.

[1] F. Esch, C. Dri, A. Spessot, C. Africh, G. Cautero, D. Giuressi, R. Sergo, R. Tommasini, G. Comelli, Rev. Sci. Instrum. 2011, 82, 53702.

[2] B. A. J. Lechner, F. Knoller, A. Bourgund, U. Heiz, F. Esch, J. Phys. Chem. C 2018, 122, 22569.

O 40.8 Tue 18:00 Poster D

In-Situ Magnesium Thin Film Nanoscale Hydrogenography — •Julian Karst, Florian Sterl, Heiko Linnenbank, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

During the hydrogenation of Magnesium (Mg), a phase change from the metallic Mg to dielectric magnesium hydride (MgH2) occurs, rendering it highly interesting for switchable optical systems. In such active systems, the nanoscale hydrogen diffusion mechanism is clearly of utmost importance, yet, so far, the details are not well understood.

To this end, we perform scattering-type scanning near-field optical microscopy to image the phase transition from Mg to MgH2 on the nanometer scale in an in-situ environment. Additionally, we perform nanoFTIR spectroscopy and identify a phonon resonance which aids in our experimental scheme. The resonance causes a very high material contrast between Mg and MgH2 in 2D near-field scattering phase images.

Our results reveal that the phase transition is nucleated at grain boundaries. From these sites, the hydrogenation front progresses into the adjoining nanocrystallites. Most interestingly, the hydrogenation seems to saturate before the entire films is hydrogenated, leaving areas of metallic Mg within the dielectric MgH2. Our results constitute an important step forward in the understanding of the hydrogen loading process in Mg and are expected to help improving the diffusion kinetics as well as the efficiency of hydrogen storage in a variety of metals.

O 40.9 Tue 18:00 Poster D

Methane clathrate hydrates study using molecular dynamics simulations — •Anoop Kishore Vatti and Laxman Kumar Kundarapu — Manipal Institute of Technology, Manipal, Karnataka, India

Gas clathrates are found copiously in permafrost region. In natural gas reservoirs or gas processing field, hydrates are formed by the chemical combination of the water and gas (precisely methane) at temperature above the freezing point of water. Gas clathrates are crystalline solids composed of water (ice) and gas (Methane/Ethane/Propane/CO2). The most common hydrate structure i.e. sI (structure I) is investigated. These cubic structure forms a combination of polyhedral cages (water) hosting the guest molecule (methane). We performed classical molecular dynamics (MD) simulations to understand the behaviour of gas hydrates using various water models (SPC/TIP3P/TIP4P) under extreme pressure. The structural properties and accuracy of the various water models be discussed.

O 41: Poster Tuesday: Nanostructures

Time: Tuesday 18:00–20:00 Location: Poster D

O 41.1 Tue 18:00 Poster D

Bridging states vs. simple droplets on prepatterned substrates: a free energy analysis — •Leon Topp and Andreas Heuer — Westfälische Wilhelms-Universität, Institut für Physikalische Chemie, 48149 Münster, Germany

Since the wetting properties of surfaces play a huge role in many technical applications, a lot of effort has been spent on the investigation of the behavior of droplets on homogenous as well as on heterogeneous surfaces. A simple model for a heterogeneous structure is a substrate which contains alternating lyophobic and lyophilic stripes. To better understand the behaviour of droplets on such surfaces we performed Monte Carlo simulations of systems with two lyophilic stripes, separated by a lyophobic one, and analyse the configurations with Markov State Modelling and Umbrella sampling to calculate free energy profiles. We determined different topological states where a drop is e.g. either placed on one of the lyophillic stripes or forms a bridge between these stripes. The weight of both configurations strongly depends on the stripe width and their mutual distance. With the resulting free energy profiles we gained phase diagrams and derived parameter regimes were a transition between the states is easily possible.

O 41.2 Tue 18:00 Poster D

Droplets on switchable substrates: a simulation study — •Leon Topp and Andreas Heuer — Westfälische Wilhelms-Universität, Institut für Physikalische Chemie, 48149 Münster, Germany

In this work the wetting of switchable surfaces is analyzed. These surfaces can change their hydropobicy due to an external stimulus like for example light of a defined wave length. To complement current experiments, it is desirable to study these systems also from a theoretical perpective. To evaluate the nonequilibrium effects resulting from the switching process, we performed Molecular Dynamic simulations where we modelled a droplet consisting of Lennard-Jones particles on a switchable surface. Here we present the impact of different switching frequencies on the droplet. In particular the (time-dependent) shape and the size of the resulting droplets are analyzed.

O 41.3 Tue 18:00 Poster D

Ion adsorption at solid-liquid interfaces — •Alina Sparenberg, Michael Paulus, Yury Forov, Susanne Dogan, Göran Surmeier, Jennifer Bolle, Mirko Elbers, Kristina Berger, Kevin Foryt, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund

The investigation of the microscopic structure of aqueous solutions is one of the important areas of modern research. In particular, the understanding of the behavior of ions at interfaces is essential for the explanation of interfacial phenomena occurring in nature and technology. A lot of pioneering work has been done to determine the interactions between ions and hydrophobic surfaces, but a complete description of the physical mechanisms for the hydrophobic interaction is still pending. Thus, we used octadecyltrichlorosilane (OTS) coated surfaces in order to study the adsorption behavior of different ions at hydrophobic solid-liquid interfaces by x-ray reflectivity. Since a first study with alkali halides indicated changes within the structure of the OTS coating that seem to scale with the ion size, this study deals with the adsorption behavior of ions with strongly varying cation sizes. For this purpose, aqueous solutions of NaBr and the ionic liquid 1-Butyl-3-methylimidazolium bromide ([BMIM][Br]) were chosen. The reflectivity experiments were performed at the beamline BL9 of the synchrotron light source DELTA in Dortmund, Germany.

O 41.4 Tue 18:00 Poster D

X-Ray Reflectivity Measurements of FeCo/TiN Magnetostructures — •Henning Vogt[1], Philipp Jordt[1], Jan-Philipp Kress[1], Niklas Wolff[2], Lorenz Kienle[2], Stefan Beierle[3], Olaf M. Magnussen[1], and Bridget M. Murphy[1] — [1]Institute of Experimental and Applied Physics, Kiel University, Leibnizstr. 19, 24098 Kiel, Germany — [2]Institute of Material Sciences, Kiel University, Kaiserstr. 2, 24143 Kiel, Germany — [3]Institute of Applied Materials – IAM-AWP, KIT Karlsruhe, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

FeCo/TiN magnetostructures are strong canidates as robust biomagnetic sensors. FeCo has desirable magnetic properties, but loses them in thick layers. By applying alternating layers of FeCo and TiN—a material known for its hardness and corrosion resistance—the FeCo is epitaxially stabilized and keeps its magnetic properties. The samples consist of hundreds of layers of a few monolayers thickness on a silicon wafer grown by magnetron sputtering. Their atomic structure has been explored using TEM to obtain local structural information and by X-ray diffraction to investigate the whole multilayer stack.

X-ray reflectivity has revealed the structure perpendicular to the surface showing that a regular layering of FeCo/TiN forms a superlattice. Sharp peaks corresponding to the layer period are observed. Further information including thickness, roughness and the electron density of each layer is obtained by modelling the reflectivity. We show that annealing the samples leads to lowering of the electron densities of the topmost layers, suggesting oxidation or atomic diffusion.

O 41.5 Tue 18:00 Poster D

One-dimensional molecular chains of Quinacridone on Ag(100) and Cu(111): STM- and SPA-LEED-investigations — •Niklas Humberg[1], Rémi Bretel[2], Alexander Eslam[1], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany — [2]University of Paris-Saclay, Institut des Sciences Moléculaires D'Orsay, France

One-dimensional molecular aggregates are of high interest because they often show specific and pronounced coupling effects for electronic excitations, e.g. in optical spectra. Here, we report a structural analysis of two such systems, quinacridone (QA) on Ag(100) and Cu(111), by STM and SPA-LEED.

On Ag(100) QA grows in parallel homochiral one-dimensional chains at room temperature (RT), forming a metastable structure. Within these chains the molecules are parallel and linked pairwise via two hydrogen bonds. The distance between neighboring chains varies with coverage. After annealing at 500 K, a two-dimensional commensurate heterochiral structure is formed. It consists of homochiral dimers forming periodically indented and closely packed chains.

On Cu(111), QA grows in similar fashion at RT. However, the structure shows more disorder than that on Ag(111). The majority of the chains are not straight and contain many kink-like defects. The high degree of disorder also becomes apparent in the SPA-LEED pattern. The observed spots smear out, yielding a highly symmetric diffraction pattern with many lines of varying intensities.

O 41.6 Tue 18:00 Poster D

Aromatic self-assembled monolayers as protective layer for silver SERS substrates — •Martha Frey[1], Christof Neumann[1], Maria Küllmer[1], Susanne Pahlow[2], Andreas Winter[1], Martin Jahn[2], Uwe Hübner[2], Dana Cialla-May[2], Karina Weber[2], Jürgen Popp[1,2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Leibniz Institute of Photonic Technology, Member of the Leibniz Research Alliance Leibniz Health Technology, 07745 Jena, Germany

Surface enhanced Raman spectroscopy (SERS) is an established technique for specific detection of fingerprint spectra of molecules at lowest concentrations. In particular, the application of silver-based SERS substrates is promising due to their favorable physical properties for enhancing Raman signals. However, the silver substrates may deteriorate with time due to oxidation. Here we present a study on preventing these unwanted changes by passivating the SERS substrates with aromatic self-assembled monolayers (SAMs). We prepare the SAMs in UHV and characterize them in situ by X-ray photoelectron spectroscopy (XPS) and ex situ by SERS. After exposing these samples for several months to ambient conditions, we conducted a comparative study by both techniques. Furthermore, we characterized the samples by scanning electron microscopy (SEM). We show an enhanced stability of the passivated substrates in comparison to the bare substrates. The presence of functional groups in the SAMs leads towards specific biochemical functionalization of the SERS substrates.

O 41.7 Tue 18:00 Poster D

Wrinkle-free centimeter-scale ultrathin alumina membranes on arbitrary substrates prepared by fast surface-energy-assisted drying — •Huanming Zhang, Min Zhou, Yang Xu, Rui Xu, Yi Wang, Zhiqiang Zeng, and Yong Lei — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693 Ilmenau

Ordered nanostructures always perform better than the disordered counterpart in many fields. Ultrathin Anodic Aluminum Oxide (AAO) membrane (UTAM) -directed fabrication is a promising technology to prepare ordered nanostructure. To transfer UTAM onto a target substrate, hydrophilic treatment or organic solvent wetting on substrate is necessary, Otherwise, a significant number of wrinkles will be generated in UTAM, and its uniformity and quality is damaged. However, widely used hydrophilic treatments, such as Oxygen plasma and Piranha solution, and organic solvent wetting are not applicable to some substrates. Moreover, the effect of the hydrophilic treatment is temporary and will be lost with time. Herein, we propose a convenient and practical technique, assisted by surface energy, to transfer UTAM onto arbitrary substrates with no observable wrinkle. Compared with surface treatments and organic solvent wetting, our method is rapid, simple, cheap, convenient and safe. In addition, the reasons behind crumpled UTAM was probed into.

O 41.8 Tue 18:00 Poster D

STM investigations on CoO_2 chains on Pt(001) — •Paula M. Weber, Chong-Heeon Park, Martin Schmitt, Matthias Vogt, and Matthias Bode — Physikalisches Institut, Lehrstuhl für Experimentelle Physik II, Universität Würzburg, Deutschland

Recently, the structural and magnetic properties of transition metal oxides (TMO) on heavy fcc(001) surfaces, such as Ir(001) or Pt(001), have attracted considerable interest [1,2]. Here, we present a spin-polarized STM investigation of CoO_2 on Pt(001). Whereas a ferromagnetic coupling along the chains was predicted for CoO_2/Ir(001) [1], it has been proposed that the CoO_2 on Pt(001)-system has an antiferromagnetic ground state [2].

Topographic STM data confirm a perfectly ordered (3×1) structural phase with a periodicity of $3a_{\mathrm{Pt}}$ between the TMO chains. Spin-resolved data were acquired by scanning with out-of-plane or in-plane polarized Cr- or Fe-coated W-tips respectively, whereby the sensitivity of each tip was characterized by test measurements on the Fe-layer on W(110). In contrast to expectations, we did not find any magnetic contrast in our SP-STM data of CoO_2/Pt(001).

We will discuss the implications of the observed structural contrasts and how the surface changes upon adsorption of residual gas from the vacuum system.

[1] P. Ferstl, *et al.*, Phys. Rev. Lett. **117**, 046101 (2016)
[2] P. Ferstl, *et al.*, Phys. Rev. B **96**, 085407 (2017)

O 41.9 Tue 18:00 Poster D

Sandwich-molecular wires: Combining cyclooctatetraene with rare- and alkaline-earth metals on Gr/Ir(111) — •Stefan Kraus[1], Ken Bischof[1], Felix Huttmann[1], Alexander Herman[2], Nico Rothenbach[2], Katharina Ollefs[2], Nicolae Atodiresei[3], Heiko Wende[2], and Thomas Michely[1] — [1]Universität zu Köln, Germany — [2]Universität Duisburg-Essen, Germany — [3]Forschungszentrum Jülich, Germany

We investigate the growth of sandwich-molecular wires, one-dimensional arrangements of alternating organic molecules and metal atoms. Here, we combine cyclooctatetraene (Cot, C_8H_8) with rare- and alkaline-earth metals in an on-surface synthesis on the inert substrate graphene/iridium(111). Recently, such wires were grown using europium (Eu), yielding crystalline islands of interlocked wires with intra-/interwire distances of 4.4Å/6.8Å. Based on the favored 2- oxidation state of Cot in this compound, we explore whether the same synthesis principle holds also for other metals releasing $2e^-$ to Cot. From the rare-earth elements we test ytterbium (Yb) and from the alkaline-earth elements barium (Ba), both favoring oxidation state 2+ in this compound. In fact, for both cases wire formation in islands is observed, with intra-/interwire distances of 4.1Å/6.4Å for Yb and 4.8Å/6.8Å for Ba which are in agreement with the slightly smaller/larger atomic radius of Yb/Ba compared to Eu. Furthermore, we accomplished to grow alloy wire islands by co-depositing Eu and Yb during synthesis.

O 41.10 Tue 18:00 Poster D

Melting behavior of FeNi nanoparticles on surfaces — •Mahboobeh Ravankhah and Mathias Getzlaff — Institute of Applied Physics, University Duesseldorf

Magnetic nanoparticles have received great attention due to their application in biomedicine and magnetic recording. The 3d bimetallic nanoparticles such as FeNi have much more complex magnetic and structural phases under different conditions. Therefore, it is important to investigate structure dependence on temperature and stoichiometry. FeNi alloy nanoparticles are prepared by a magnetron sputtering source and an Arc Cluster Ion Source (ACIS). Two different FeNi alloys are used: high purity Fe0.50Ni0.50 and Fe0.75Ni.25. All nanoparticles are prepared under UHV condition on W (110) surface, therefore contaminations are avoided. We report on the influence of different parameters like size of nanoparticles, stoichiometry and annealing temperature on the melting behavior. Particle's size, shape and structure will be investigated by Transmission Electron Microscopy (TEM), Scanning

Tunneling Microscopy (STM) and Low Energy Electron Diffraction (LEED).

O 42: Poster Tuesday: Organic Molecules on Inorganic Surfaces

Time: Tuesday 18:00–20:00 Location: Poster D

O 42.1 Tue 18:00 Poster D

LT-UHV-STM Investigations on Various Supramolecular Structures of Benzylnaphthoic Diimides Adsorbed on an Au(111)-Surface — •Bertram Schulze Lammers[1,2], René Ebeling[2], Elena Dirksen[3], Thomas J. J. Müller[3], and Silvia Karthäuser[2] — [1]Institute of Physics and Center for Nanotechnology, University of Münster, Germany — [2]Peter Grünberg Institut (PGI-7) and JARA-FIT, Forschungszentrum Jülich GmbH, Germany — [3]Institut für Organische Chemie und Makromolekulare Chemie, Heinrich-Heine-Universität Düsseldorf, Germany

By means of the LT-UHV-STM technique we investigated 2,7-dibenzyl 1,4,5,8-naphthalenetetracarboxylic diimide (BNTCDI), which consists of a naphthalene diimide (NDI) backbone and two benzyl groups. On a Pt(111)-surface it showed the formation of an effective transport path via hybrid BNTCDI/Pt d-states [1]. For a deeper understanding we investigated BNTCDI on an Au(111)-surface, where a weak physisorption is expected. As a result, we obtained one- and two-dimensional supramolecular structures. Orbital-resolved STM imaging allows us to identify intramolecular hydrogen bonds between the NDI-backbones as the driving force for the one-dimensional arrangements on step-edges. The two-dimensional structures on the terraces emerge as ordered and disordered molecular double layers. Locally resolved STS measurements reveal the characteristic electronic properties of BNTCDI and the influence on these by different substrate coupling strengths. In particular, we identify a LUMO-shift and an edge-state coupling as prominent adsorption driven influences. [1] DOI: 10.1021/acs.jpcc.7b09911

O 42.2 Tue 18:00 Poster D

Metalation of phthalocyanines on semimetal surfaces and the manifestation of interfacial electronic structures — Jinbang Hu[1,2], Zhengde Zhang[1], Kongchao Shen[1,3], Zhaofeng Liang[1,2], Haoliang Sun[1,2], Jinpin Hu[1,2], Gengwu Ji[1], Xingyu Gao[1], Ping Huai[1], Zhiyuan Zhu[1], Zheng Jiang[1], Han Huang[4], •Frode Strand[5], Rajesh Chellappan[5], Justin Wells[5], Bo Song[6], and Fei Song[1] — [1]IPAT and SSRF, Shanghai. Institute of Applied Physics, SINAP CAS, Shanghai, China — [2]UCAS, Beijing, China — [3]Department of Physics, ZHU, Hangzhou, China — [4]School of Physics and Electronics, CSU, Changsha, China — [5]Center of Quantum Spintronics and Department of Physics, NTNU, Trondheim, Norway — [6]USST, Shanghai, China

On-surface engineering of supramolecular structures has attracted much interest during past decades, for example, the manipulation of metal coordination, hydrogen bonding and so on. However, organic nanostructures coordinated by group-V semimetals have generally not been reported. Specifically, synthesis of non-transition metal phthalocyanines (PC) are scarcely discussed in the literature. Here we will report on the on-surface metalation of H2-PC to form Bi-PC (and similarly Sb-PC). The formation of Bi-PC is studied using XPS and LEED, and the interfacial electronic states are studied using UPS. Our findings confirm the feasibility of on-surface metalation of H2PC to form non-transition-metal PCs which are otherwise difficult to synthesise.

O 42.3 Tue 18:00 Poster D

Exciting vibrons in both frontier orbitals of a single hydrocarbon molecule on graphene — •Alexander Mehler[1], Nicolas Néel[1], Marie-Laure Bocquet[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, Ilmenau, Germany — [2]Department of Chemistry, UMR ENS-CNRS-UPMC 8640, Ecole Normale Supérieure, Paris, France

Vibronic excitations in molecules are key to the fundamental understanding of the interaction between vibrational and electronic degrees of freedom. In order to probe the genuine vibronic properties of a molecule even after its adsorption on a surface appropriate buffer layers are of paramount importance. Here, vibrational progression in both molecular frontier orbitals is observed with submolecular resolution on a graphene-covered metal surface using scanning tunnelling spectroscopy. Accompanying calculations demonstrate that the vibrational modes that cause the orbital replica in the progression share the same symmetry as the electronic states they couple to. In addition, the vibrational progression is more pronounced for separated molecules than for molecules embedded in molecular assemblies. The entire vibronic spectra of these molecular species are moreover rigidly shifted with respect to each other. This work unravels intramolecular changes in the vibronic and electronic structure owing to the efficient reduction of the molecule-metal hybridization by graphene.

O 42.4 Tue 18:00 Poster D

Promoted exchange reaction between alkanethiolate self-assembled monolayers and an azide-bearing substituent — Rui Yan[1], Loïc Le Pleux[2], Marcel Mayor[2,3], and •Michael Zharnikov[1] — [1]Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [2]University of Basel, Department of Chemistry, CH-4056 Basel, Switzerland — [3]Forschungszentrum Karlsruhe GmbH, Institute for Nanotechnology, 76021 Karlsruhe, Germany

The possibility of ultraviolet-light-promoted exchange reaction between the primary alkanethiolate (AT) self-assembled monolayers (SAM) and an azide-functionalized substituent (12-Azido-1-dodecanethiol, C12N3), capable of click reaction with ethynyl-bearing species, is demonstrated. This reaction resulted in the mixed AT/C12N3 films, with the portion of C12N3 precisely controlled by selection of a suitable UV dose. As the primary matrix, either non-substituted or oligo(ethylene glucole) (OEG) substituted AT SAMs were used, targeting mixed SAMs of chemical and biological significance. The surface density of the chemically active azide groups embedded in the non-reactive primary matrix could be precisely varied. For the OEG-AT/C12N3 films, this resulted in the preparation of templates for specific protein adsorption, comprising biotin-bearing moieties embedded in the protein-repelling OEG-AT matrix. The entire approach was extended to lithography, relying on a commercial maskless UV lithography setup.

O 42.5 Tue 18:00 Poster D

Revealing spectroscopic signatures of molecule-metal interaction: A computational core-level spectroscopy study — •Samuel J. Hall and Reinhard J. Maurer — Department of Chemistry, University of Warwick, Coventry, United Kingdom

Core-level spectroscopy, both x-ray absorption (XAS) and photoemission (XPS), represents an immensely important tool for the characterisation of complex hybrid organic-inorganic interfaces. The information on these interactions is often hidden in a convolution of spectroscopic signatures that is affected by initial state effects (e.g. chemical bonding) and final state effects (e.g. molecule-metal charge-transfer and hybridisation) alike. First-principles simulation of core-level spectra enables us to disentangle these effects and offers a systematic assessment of varying molecule-metal interaction strength and its spectral manifestation. On the examples of small conjugated organic molecules and aromatic carbon nanostructures at single-crystal metal surfaces such as Cu(111), Ag(111), and Pt(111), we investigate the signatures of molecule-metal bonding by simulating near-edge X-ray absorption fine-structure (NEXAFS) and XPS spectra. Calculations were carried out using dispersion-inclusive Density Functional Theory calculations using the transition potential method. [1,2] Using orbital-projection techniques, we are able to provide a full spectral decomposition in terms of initial and final states. In combination with a charge and structure analysis, we arrive at a detailed picture of how molecular composition and metal reactivity affect core-level spectra. [1] JCP **146**, 214701 (2017), [2] PRB **58**, 8097 (1998)

O 42.6 Tue 18:00 Poster D

Electronic Structure of decoupled molecules: 1,2;8,9-dibenzopentacene on h-BN on Pt(111) — •Maximilian Schaal, Felix Otto, Bernd Schröter, Roman Forker, and Torsten Fritz — Friedrich Schiller University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena

The strong hybridisation of molecules on metal single crystals causes a strong change of the structural and electronic proporties. Insulating interlayers like 2D hexagonal boron nitride (h-BN) can be used to study the undisturbed properties of decoupled molecular layers. For this purpose we studied the change of the electronic structure of 1,2;8,9-dibenzopentacene (trans-DBPen) molecules upon adsorption on h-BN/Pt(111). The h-BN monolayer was grown by thermal dehydrogenation of borazine on Pt(111). The layer quality was determined by x-ray photoelectron diffraction (XPD) and low energy electron diffraction (LEED). The thickness of the trans-DBPen layer was controlled by in-situ differential reflectance spectroscopy (DRS). The electronic structure of this organic-inorganic heterostructure was observed with ultraviolet and x-ray photoelectron spectroscopy (UPS and XPS) and compared to the electronic structure of bare h-BN on Pt(111) and trans-DBPen directly on Pt(111). By measuring the band structure it was possible to identify several molecular states. Furthermore, the highest occupied molecular orbital (HOMO) was investigated by measuring the photoelectron momentum maps (PMMs). Finally the results show the desired effect of decoupled trans-DBPen molecules on h-BN/Pt(111).

O 42.7 Tue 18:00 Poster D

Understanding the Mechanism of Metalation at Porphyrin/CoO(111) Interfaces with Photoemission Spectroscopy — •Can Wang, Ruimei Wang, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Understanding the electronic structure between porphyrins and metal oxide interfaces is vital for the rational design of functional molecular architectures [1, 2]. Well-ordered thin layers (∼5 ML) of rock-salt structure CoO(111) are expitaxially grown on Ir(100) [3, 4]. Here, we study the electronic properties of porphyrin (2H-DPP and 2H-TPP) films adsorbed on CoO(111) surface by means of photoemission spectroscopy methods. We observed the direct metalation between porphyrin molecules (∼1 ML) and CoO(111) interface at room temperature with N 1s core-level shifts obtained by using XPS measurements. The formation of Co-DPP or Co-TPP lead an additional electronic state located ∼0.4 eV below the Fermi level in UPS spectrum. The UV photoemission data, obtained from monolayer films of 2H-DPP and 2H-TPP also show a large decrease of work function.

[1] W. Auwärter et al., Nat. Chem. 7, (2015) 105.

[2] G. Di Filippo et al., J. Chem. Phys. 146, (2017) 064702.

[3] K. Heinz et al., J. Phys.: Condens. Matter 25, (2013) 173001.

[4] S. Otto and Th. Fauster, J. Phys.: Condens. Matter 28, (2016) 055001.

O 42.8 Tue 18:00 Poster D

Influence of Porphyrinoid Ring Contraction: Transition Metal Corroles — •Jan Herritsch[1], Jan-Niclas Luy[1], Malte Zugermeier[1], Falk Niefind[1], Qitang Fan[1], Martin Schmid[1], Peter Schweyen[2], Martin Bröring[2], Ralf Tonner[1], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Institut für Anorganische und Analytische Chemie, TU Braunschweig, Germany

Porphyrin complexes are well studied model systems for surface functionalization. Their reactivity can be controlled by variation of the ligand skeletal structure and the central atom. The related corroles represent contracted porphyrins. Contrary to the formally dianionic porphyrins, they usually act as trianionic ligands and stabilize higher oxidation states of the central atom. Here, we present the on-surface synthesis and characterization of different transition metal corroles (Fe, Co, Ni) on the Ag(111) surface and compare them with the corresponding porphyrins. Thus, we have studied the influence of ring contraction on the electronic structure and adsorbate-substrate interactions. The electronic states of the cobalt and nickel corrole complexes were found to be very similar to those of the corresponding porphyrins. This can partly be explained by the redox non-innocent behavior of the corrole ligand. In case of iron the corrole and porphyrin complexes differ from each other in their electronic state according to XP and NEXAFS spectra. These findings can be observed in the substrate-decoupled multilayer as well as in the monolayer and a higher oxidation state of the iron corrole was verified by UPS.

O 42.9 Tue 18:00 Poster D

Surface Chemical Bond of Alternant vs. Non-Alternant Aromatic Isomers — •Ruppenthal Lukas, Bendedikt P. Klein, Jan Herritsch, Stefan R. Kachel, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Metal/organic interfaces have a large impact on the performance of organic-electronic devices. The detailed understanding of their chemical, electronic and geometric structure is therefore important for the further technological development. Many common organic semiconductors contain aromatic structures with alternant topologies, whereas non-alternant alternatives have found far less interest. Here, we compare naphthalene as an alternant aromatic molecule to azulene as its non-alternant isomer, both on Cu(111), using PES, NEXAFS, TPD, STM, and LEED. With the same approach, we compare the larger aromatic compounds pyrene and its isomer dicyclopenta[*ef,kl*]heptalene (azupyrene), which is also important as a model for the Stone-Wales defects in graphene. Related studies on organometallic sandwich complexes include bis(benzene)chromium and the corresponding non-alternant cyclopentadienyl-cycloheptatrienyl-chromium. In all cases, we find that the non-alternant structure forms a stronger bond to the metal surface than its alternant counterpart. The main reason for this is that the non-alternant species have a smaller HOMO-LUMO gap, which makes them both better donors and better acceptors compared to the alternant species. The resulting effects on the electronic and geometric structure will be discussed on the basis of DFT calculations.

O 42.10 Tue 18:00 Poster D

Orbital Imaging of Pentacene Bilayers on Ag(110) — •Kiana Baumgärtner[1], Manuel Grimm[1], Christian Metzger[1], Martin Graus[1], Matteo Jugovac[2], Giovanni Zamborlini[2], Vitaliy Feyer[2], Achim Schöll[1], and Friedrich Reinert[1] — [1]Julius-Maximilians-Universität Würzburg, Experimental Physics VII, 97074 Würzburg, Germany — [2]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-6), 52425 Jülich, Germany

Pentacene, a planar organic molecule being widely used in organic electronic devices, is known to form well-ordered single layers when evaporated atop Ag(110). Due to substrate-molecule interactions, the molecules of the first layer will align themselves flat-lying and commensurately along the [001] direction of the substrate. When adding a second layer of molecules, the orientation of growth is increasingly determined by intermolecular forces resulting in a tilt angle of the first layer away from the substrate surface and an even larger tilt angle in the second layer. To evaluate the exact angles of the individual layers, photoelectron momentum maps were recorded with a photoemission electron microscope in k-space imaging mode (kPEEM) at a synchrotron radiation source. The obtained momentum maps contain information on the orientation of the investigated orbital and thus, a comparison of the experimental data with simulated intensity distributions for different sample geometries allowed for a verification of the tilt angle with an accuracy of about 1°.

O 42.11 Tue 18:00 Poster D

Rubber-modified polybenzoxazine-based materials for surface coating applications — •Eugene B. Caldona[1], Al Christopher C. De Leon[2], Bryan B. Pajarito[3], and Rigoberto C. Advincula[2] — [1]Department of Chemistry, Mississippi State University, Mississippi State, MS 39762, USA — [2]Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, OH 44106, USA — [3]Department of Chemical Engineering, University of the Philippines Diliman, Quezon City 1101, Philippines

This work demonstrates the preparation of rubber-modified polybenzoxazine (PBZ) where additives such as graphene oxide (GO), polyaniline (PANI), and nano-silica (SiO2) are added separately and the resulting materials are used as surface coatings. PBZ is known for its near-zero shrinkage upon polymerization, chemical resistance, and good dielectric, thermal, and mechanical properties. PBZ has low surface free energy and low water absorption making it an excellent candidate for protective coating study. GO is added because of its ability to form a tortuous path leading to reduced permeability and enhanced barrier property. PANI, a conducting polymer, promotes passivation by forming a thin layer of metal oxides that further increase the anodic protection of the coating. Lastly, on top of providing superior corrosion protection, nano-SiO2 introduces surface roughness that results in excellent anti-wettability, anti-icing, self-cleaning property, and superoleophilicity. Combined with good thermal and adhesion properties, the rubber-modified PBZ with different additives are said to be very promising surface coating materials for a variety of applications.

O 42.12 Tue 18:00 Poster D

Growth Inhibition of <i>P. Fluorescens<i> Biofilms by Ag/Teflon-Like Thin Films: A Comparative Morphological and Spectroscopic Study — •Maria Chiara Sportelli[1], Ruggiero Quarto[1], Erhan Tütüncü[2], Antonio Valentini[3], Christine Kranz[2], and Nicola Cioffi[1] — [1]Chemistry Department, University of Bari, V. Orabona, 4-70126 Bari, Italy. — [2]Institute of Analytical and Bioanalytical Chemistry, Ulm University, Albert Einstein Allee, 11 * 89081 Ulm, Germany — [3]Dipartimento Interateneo di Fisica *M. Merlin*, University of Bari, V. Orabona, 4-70126 Bari, Italy

Ag-Teflon-like (Ag-CFx) composites were obtained by ion beam cosputtering of polytetrafluoroethylene (PTFE) and Ag targets. AgNPs are already used as antimicrobials in health industry, for food storage, in environmental applications. There is an increasing need of anti-biofouling surfaces and materials, to prevent biofilm formations. Biofilms, i.e. colonies of microorganisms embedded in an extracellular polymeric matrix, are a major cause of healthcare-associated infections, since bacteria are highly resistant to antimicrobials. In this perspective, the inhibition of biofilm growth is a crucial issue in the prevention of bacterial infections. In the present study, Ag-CFx composites were characterized by TEM, AFM, XPS and AAS. They were also deposited onto ZnSe ATR crystals. This approach allowed real-time monitoring of P. fluorescens biofilm growth and inhibition induced by the antimicrobial coating. These findings were corroborated by AFM imaging of bacteria incubated on Ag-CFx films.

O 42.13 Tue 18:00 Poster D

Electrospray Ion-Beam Deposition: UHV-deposition of nonvolatile molecules — •Sabine Abb[1], Hannah Ochner[1], Sven Szilagyi[1], Stephan Rauschenbach[1,2], and Klaus Kern[1,3] — [1]Max Planck Insitute for solid state research, Stuttgart, Germany — [2]University of Oxford, UK — [3]Ecole Polytechnique Fédérale de Lausanne, CH

The standard technique to deposition molecules in ultra-high vacuum (UHV) is evaporation/sublimation. However, evaporation is limited to volatile molecules, e.g. molecules that can be brought in the gas phase without decomposition by heating. Electrospray Ion-Beam deposition gives access to non-volatile molecules of different classes, such as biomolecules, dyes and other complex molecules and therefore expands the range of samples in UHV. Employing the possibility of mass spectrometry and subsequent mass filtering, highly pure samples can be fabricated.

In this poster, we will show an overview of the recent work performed with our home-built electrospray ion-beam deposition instrument in conjuction with STM.

O 43: Poster Tuesday: Electronic Structure

Time: Tuesday 18:00–20:00 Location: Poster D

O 43.1 Tue 18:00 Poster D

Studying the type-II Weyl semimetal candidate *Td*-WTe$_2$ with two-photon photoemission — •Petra Hein[1], Stephan Jauernik[1], Yulin Chen[2], Lexian Yang[2], Binghai Yan[3], Claudia Felser[3], and Michael Bauer[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, Germany — [2]Physics Department, Tsinghua University, Beijing, China — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Laser-based angle-resolved photoemission spectroscopy (ARPES) and two-photon photoemission (2PPE) are combined to investigate the near-E$_F$ electronic structure of the type-II Weyl semimetal candidate WTe$_2$.

Using a widely tunable femtosecond laser system, we are able to access a variety of both occupied and unoccupied electronic states. Initial, intermediate and final states can be clearly distinguished via their characteristic peak shift in dependence of the photon energy. Photon-energy scans in conventional ARPES studies of three-dimensional systems are typically used to determine the k$_z$ dispersion of the occupied band structure. Here we show that in an analogous manner 2PPE is capable of probing the k$_z$ dispersion of unoccupied bands between E$_F$ and the vacuum level. The results are compared to different band structure calculations and current ARPES studies of WTe$_2$.

O 43.2 Tue 18:00 Poster D

Drumhead Surface States in ZrSiTe — •Andreas Topp[1], Lukas Müchler[2], Raquel Queiroz[3,1], Bettina V. Lotsch[1], Leslie M. Schoop[4], and Christian R. Ast[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, DEU-70569 — [2]Flatiron Institute, New York, USA-10010 — [3]Weizmann Insitute of Science, Rehovot, ISR-7610001 — [4]Department of Chemistry, Princeton University, Princeton, USA-08544

ZrSiS, ZrSiTe and related compounds have become of increased interest in recent years. As members of space group 129, their crystal structure contains nonsymmorphic symmetry elements in combination with a square-net lattice of atoms. While the nonsymmorphic symmetry is responsible for band crossings at high-symmetry points that are not affected by spin-orbit coupling, the square net produces a Dirac line node forming a diamond-like structure in the first Brillouin zone. ARPES measurements showed additional surface states in ZrSiS that could be explained in the framework of reduced surface symmetry [1]. Here, we focus on the isostructural compound ZrSiTe, which shows an even more complicated surface band structure and explain the emergent surface bands in the context of topological drumhead surface states [2].

[1] Topp et al., Phys. Rev. X 7, 041073 (2017).
[2] Y.-H. Chan et al., Phys. Rev. B 93, 205132 (2016).

O 43.3 Tue 18:00 Poster D

STM-Investigations of Re(0001) suface states — •Johannes Regel[1], Torge Mashoff[1], Jürgen Braun[2], Hubert Ebert[2], and Hans-Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz — [2]Department Chemie, Ludwig Maximilians-Universität, München

Due to the broken symmetry, the electronic structure of surfaces can differ significantly from the bulk structure. In case of strong spin-orbit coupling, as given in rhenium, this can lead to Rashba spin splitting of the electronic states. Although the strong spin momentum should forbid backscattering, the rhenium surface shows standing waves in the local density of states originating from defects and step edges. We investigate the electronic states of the Re(0001) surface using low temperature scanning tunneling microscopy and spectroscopy. Differential conductivity measurements lead to an energy-dependent analysis of the wavelength, phase and damping of these states. Additionally, we use molecular beam epitaxy to deposit sub-monolayer gold and nickel islands onto the Re-surface and study their influence on the measurements as well as the pseudomorphic growth of these metals. Our results are compared with one-step model calculations of the electronic structure of rhenium and show good agreement.

O 43.4 Tue 18:00 Poster D

On superconducting properties of clean Nb(110) surface and its magnetic adatom-induced Yu-Shiba-Rusinov states — •Artem B. Odobesko, Stefan Wilfert, Robin Boshuis, and Matthias Bode — Physikalisches Institut, Universität Würzburg, Am Hubland, Würzburg, Germany

We have studied cleaning procedures of Nb(110) by low-energy electron diffraction, Auger electron spectroscopy, and scanning tunneling microscopy and spectroscopy. Our results show that the formation of a surface-near impurity depletion zone is inhibited by the very high diffusivity of oxygen in the Nb host crystal. Oxygen can be removed from the surface by heating the crystal to $T \sim 2400°C$. Tunneling spectra measured on the clean Nb(110) surface exhibit a sharp conductance peak in the occupied states at an energy of about -450 meV. The clean Nb(110) surface is superconducting with a gap width and a critical magnetic field strength in good agreement to the bulk value. Spatially resolved spectra take in an external magnetic field show a zero-bias anomaly in the vortex core. We will discuss the potential of the Nb(110) surface to serve as a platform for Yu-Shiba-Rusinov bound states inside the superconducting gap when magnetic impurities induce a pair-breaking scattering potential for Cooper pairs [1]. The adsorption site–dependence of the Yu-Shiba-Rusinov states will be explored by atomic manipulation.

[1] B.W. Heinrich, J.I. Pascual, K.J. Franke, Prog. Surf. Sci. textbf93, 1 (2018).

O 43.5 Tue 18:00 Poster D

Spectroscopic signatures of single molecules and their aggregates in the presence of a dielectric surface — •Meral Ari, Oliver Stauffert, and Michael Walter — Institute of Physics, University of Freiburg, Freiburg, Germany

Polycyclic aromatic hydrocarbons promise to be attractive candidates for materials to build the next generation of optoelectronic devices. In order to be able to utilize them at maximum yield, understanding their electronic structure and optical properties is essential. Hereby we are especially interested in acenes. We describe their electronic structures with density functional theory (DFT) and excited state properties with time-dependent density functional theory (TDDFT). Experimentally observed spectroscopic shifts are determined from the effect of the permittivity of the neon surface in a joined effort with the macroscopic QED group of S. Buhmann. The dielectric constant of the neon surface is calculated by using different ab-initio methods and their effects are compared.

O 43.6 Tue 18:00 Poster D

A one-dimensional hole gas in monolayer MoS_2 — •Clifford Murray[1], Wouter Jolie[1,2], Joshua Hall[1], Arkady Krasheninnikov[3,4], Carsten Busse[1,2,5], Hannu-Pekka Komsa[3], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [3]Department of Applied Physics, Aalto University School of Science, Aalto, Finland — [4]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [5]Department Physik, Universität Siegen, Germany

We epitaxially grow high-quality monolayer molybdenum disulfide (ML-MoS_2) on graphene on Ir(111), which is close to freestanding on this substrate [1]. We probe its electronic structure with low temperature scanning tunnelling spectroscopy.

The valence band is found to undergo stepwise bending at line defects such as 4|4E-type mirror twin boundaries (MTBs) and flake edges. Localised charge in these defects causes an upwards bending of the bands in the surrounding ML-MoS_2 semiconductor. This is experienced particularly strongly in the valence band, and leads to a 1D confinement of the charge carriers (holes) perpendicular to the defect. By contrast, the effect is not seen at 4|4P MTBs, the MTB type commonly present in the analogous $MoSe_2$ monolayer. We seek to understand and describe the observed behavior with the help of density functional theory.

[1] Hall, J. et al., 2D Mater. 5, 025005 (2018)

O 43.7 Tue 18:00 Poster D

Spin effects in the unoccupied electronic structure of Ir(111) and graphene/Ir(111) — •Fabian Schöttke, Katharina T. Ritter, Anke Beck-Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

The electronic structure of iridium surfaces is of interest with respect to spin-orbit interaction at surfaces of heavy elements. Especially the Ir(111) surface is the subject of numerous investigations because it is well suited as a substrate for graphene [1]. A two-photon-photoemission study on graphene/Ir(111) using circularly polarized light reports a Rashba-type spin splitting of the image-potential state [2]. However, this result is put into question by another study [3].

We present an inverse-photoemission study with spin resolution on the unoccupied electronic states of Ir(111) and graphene/Ir(111). We address the spin dependence of the image-potential states for the bare Ir(111) surface and the graphene-covered surface in order to examine the interaction of the substrate with the graphene overlayer.

[1] Varykhalov *et al.*, Phys. Rev. Lett. **108**, 066804 (2012).

[2] Tognolini *et al.*, Phys. Rev. Lett. **115**, 046801 (2015).

[3] Arafune *et al.*, Prog. Surf. Sci. doi:10.1016/j.progsurf.2018.08.001.

O 43.8 Tue 18:00 Poster D

Investigation of honeycomb Na_2IrO_3 surface structures by functionalized STM and STS probes — •Thomas Dziuba[1], Ina Pietsch[2], Philipp Gegenwart[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Lehrstuhl für Experimentalphysik VI, Universität Augsburg, Germany

Na_2IrO_3 is a prototypical Kitaev material in the iridate family, consisting of alternating stacks of negatively charged honeycomb Ir_2NaO_6 layers and positively charged hexagonal Na_3 layers [1]. In addition to its frustrated magnetic bulk properties, Na_2IrO_3 has also been discussed as host of topological electronic surface states. However, since most studies focus on bulk magnetic properties, information on the surface electronic structure is still rather limited. We report a thorough study of the structural and electronic properties of in-situ cleaved surfaces by atomic resolution scanning tunneling microscopy and spectroscopy. Based on our previous study of surface reconstructions [2], we now concentrate our attention on a detailed investigation of the differences between the bulk and surface electronic properties. We deeply study the influence of alkali metal functionalized tips and report the interrelation between surface reconstructions, the local electronic structure and the tip status.

Work supported by DFG through SPP 1666 (Topological Insulators).

References:

[1] Y. Singh and P. Gegenwart, Phys. Rev. B 82, 064412 (2010)

[2] F. Lüpke et al., Phys. Rev. B 91, 041405(R) (2015)

O 43.9 Tue 18:00 Poster D

Evidence for Conducting Na_2IrO_3 Surfaces prepared in UHV — •Sarah Maamar[1], Thomas Dziuba[1], Ina Pietsch[2], Philipp Gegenwart[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Lehrstuhl für Experimentalphysik VI, Universität Augsburg, Germany

Honeycomb iridate Na_2IrO_3 attracts considerable interest as prototype material for the study of the Kitaev interaction [1]. However, first-principles-derived tight-binding model calculations have also proposed topologically nontrivial electronic behaviour in this system, namely 2D Quantum Spin Hall [2] or 3D correlated topological insulator [3] states. Experimental evidence for this is still missing, possibly because of the high reactivity of Na_2IrO_3, leading to rapid degradation of its surface. To overcome this problem, we cleave single crystals in ultra-high vacuum (UHV), evaporate gold contacts and study the electrical conductivity as function of temperature between 100 K and 260 K without breaking the UHV conditions. Linear I-V curves prove ohmic contacts. In contrast to previous resistivity measurements, which displayed insulating behaviour [4], our data indicate a saturation of the resistance at low temperature, i.e. a finite conductivity at 100 K. This work is supported by the DFG through the SPP 1666 (Topological Insulators).

[1] S.M. Winter et al., J. Phys.: Condens. Matter 29, 493002 (2017).

[2] A. Shitade et al., Phys. Rev. Lett. 102, 256403 (2009).

[3] C.H. Kim et al., Phys. Rev. Lett. 108, 106401 (2012).

[4] Y. Singh and P. Gegenwart, Phys. Rev. B 82, 064412 (2010).

O 43.10 Tue 18:00 Poster D

Tunable Surface Band Inversion in Black Phosphorous — •Klara Volckaert[1], Deepnarayan Biswas[1], Brian Kiraly[2], Søren Ulstrup[1], Charlotte Sanders[3], Marco Bianchi[1], Alexander Khajetoorians[2], and Philip Hofmann[1] — [1]Aarhus University, Aarhus, Denmark — [2]Radboud University, Nijmegen, The Netherlands — [3]Central Laser Facility, Harwell, United Kingdom

Black phosphorous is a semiconductor that is gaining interest due to its tunable bandgap, which is thought to lead to an anisotropic Dirac semimetal upon critical doping with alkalis. Therefore this material could prove relevant to electronic and optoelectronic devices. Here we study the effect of potassium doping on bulk black phosphorous that leads to an elliptical electron-like pocket appearing. The nature of these bands is deduced using the k_z dispersion acquired by means of angle-resolved photoemission spectroscopy (ARPES). Curiously, at high levels of potassium deposition, electron-like states emerge below the Fermi level that have not previously been reported.

O 43.11 Tue 18:00 Poster D

Electronic properties of potassium-doped black phosphorus on the atomic scale — Brian Kiraly, •Elze Jantien Knol, Daniel Wegner, and Alexander Ako Khajetoorians — Scanning Probe Microscopy, Radboud University, Nijmegen, the Netherlands

In 2015 it was proposed that by applying a surface electric field gradient to few-layer black phosphorus, the material can be tuned from a moderate-gap semiconductor into a band-inverted semimetal [1]. Experimentally, it was shown that such a transition can be achieved by adding potassium atoms to the surface [2]. Since then there has been interest in the electronic properties of the surface of black phosphorus and the role of potassium. Here, utilizing low-temperature scanning tunneling microscopy and spectroscopy, we probe the variations in the electronic properties of black phosphorus, with varying surface coverage of potassium at the atomic scale. We discuss the changes to both the band-gap and Fermi energy, in the presence of surface doping. Moreover, we present the effect of charge-mediated interactions on the atomic distribution of potassium atoms, and relate this to the electrostatic screening of black phosphorus.

[1] Q. Liu, X. Zhang, L. B. Abdalla, A. Fazzio, A. Zunger. Nano Lett. 15 (2), 2015.

[2] J. Kim, S. S. Baik, S. H. Ryu, Y. Sohn, S. Park, B. G. Park, J. Denlinger, Y. Yi, H. J. Choi, K. S. Kim. Science 349 (6249), 2015.

O 44: Poster Tuesday: Spins and Magnetism

Time: Tuesday 18:00–20:00 Location: Poster D

O 44.1 Tue 18:00 Poster D

Yu-Shiba-Rusinov States of iron dimers on 2*H*-NbSe$_2$ — •Jannik Steinborn[1], Eva Liebhaber[1], Gaël Reecht[1], Sebastian Rohlf[2], Kai Rossnagel[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

A magnetic impurity absorbed on a superconductor leads to bound states (called Yu-Shiba-Rusinov (YSR) states) in the superconducting energy gap. These states are caused by exchange scattering between Cooper pairs and the magnetic impurity. 2*H*-NbSe$_2$ is a transition metal dichalcogenide with Van-der-Waals coupled layers. In this material superconductivity and a charge density wave (CDW) coexist at low temperatures.

Here, we investigate the YSR states of iron dimers on the surface of 2*H*-NbSe$_2$ with low temperature scanning tunneling microscopy and spectroscopy. We examine the coupling of the YSR states of the two iron atoms and the influence of the CDW.

O 44.2 Tue 18:00 Poster D

Hyperfine fields of magnetic adatoms on MgO/Ag(001) — •Sufyan Shehada, Manuel dos Santos Dias, Filipe Souza Mendes Guimarães, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

The hyperfine interaction couples the atomic nucleus to the surrounding electrons. Nuclear spin states tend to have a very long lifetime, and hold great promise as building blocks for quantum computers. Recently, the hyperfine splitting of the electron spin resonance peak was experimentally detected for Fe and Ti adatoms on MgO/Ag(001) [1]. In this contribution, we report on first-principles calculations of the hyperfine field [2] for a series of magnetic adatoms both on Ag(001) and on MgO/Ag(001) surfaces. We analyze the trends with respect to the type of adatom and its local surface environment, and explore the connection to the stability of the electronic spin states.

This work was supported by the Palestinian-German Science Bridge BMBF program and the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator Grant No. 681405-DYNASORE).

[1] P. Willke *et al.*, Science **362**, 336–339 (2018)
[2] S. Blügel *et al.*, Phys. Rev. B **35**, 3271 (1987)

O 44.3 Tue 18:00 Poster D

Kondo effect of a singly occupied molecular orbital in bis(phthalocyaninato)-dysprosium double decker molecules — •Timo Frauhammer[1], Gabriel Derenbach[1], Svetlana Klyatskaya[2], Eufemio Moreno-Pineda[2], Mario Ruben[2], and Wulf Wulfhekel[1,2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Germany

Double decker bis(phthalocyaninato)-dysprosium single molecule magnets adsorbed on Au(111) have been investigated using low temperature STM. No direct magnetic signal by the 4f electrons could be detected in STS. Interestingly, all molecules adsorbed on step edges show a clear Kondo resonance on the ligands with a Kondo temperature of about 4 K. Some molecules arranged in islands show the same behaviour. This indicates an odd number of electrons residing in the molecular orbitals of the ligands. Assuming there is a strong enough exchange coupling between the unpaired spin on the ligands and the 4-f angular momentum of the Dy central ion, the observed Kondo effect might be used as a means to indirectly address the 4-f magnetic moment.

O 44.4 Tue 18:00 Poster D

Element-Specific Magnetism of Rare-Earth-Cyclooctatetraene Nanowires — •Alexander Herman[1], Stefan Kraus[2], Nico Rothenbach[1], Katharina Ollefs[1], Jan Dreiser[3], Thomas Michely[2], and Heiko Wende[1] — [1]Universität Duisburg-Essen and CENIDE, Lotharstr. 1, 47057 Duisburg — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, 50937 Köln — [3]Swiss Light Source, Paul Scherrer Institut, Forschungsstrasse 111, CH-5232 Villigen

The analysis of the magnetic coupling and the magnetic anisotropy of localized 4f magnetic moments connected via organic ligands in molecular networks is a highly topical field of research owing to potential applications in organic spintronics. Our on-surface synthesis method allows us to synthesize sandwich-molecular nanowires that consist of alternating ring-like cyclooctatetraene (Cot) molecules and varying rare-earth ions as well as other phases of rare-earth-Cot compounds. The electronic and magnetic properties of these compounds were studied by XAS, XMCD and XLD accompanied by a theoretical approach based on multiplet calculations. The systems show, depending not only on the ligand, but also on the underlying substrate, varying magnetic coupling and magnetic anisotropies. We acknowledge financial support by DFG through the project WE 2623/17-1.

O 44.5 Tue 18:00 Poster D

On-surface chemistry of manganese corroles on Ag(111) — •Hazem Aldahhak[1], Reza Kakavandi[2], Mateusz Paszkiewicz[2], Wolf Gero Schmidt[1], Johannes V. Barth[2], Timur Biktagirov[1], Wolfgang Schöfberger[3], Eva Rauls[4], Florian Klappenberger[2], and Uwe Gerstmann[1] — [1]Department of Physics, Paderborn University, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Physics Department E20, Technical University of Munich, James-Franck-Strasse 1, 85748 Garching, Germany — [3]Institute of Organic Chemistry, Johannes Kepler University, Altenberger Strasse 69, 4040 Linz, Austria — [4]Institutt for Matematikk og Fysikk, University of Stavanger, 4036 Stavanger, Norway.

Corroles are tetrapyrrole macrocycles with promising applications in various fields of science. Here, we present a multi-technique strategy based on density functional theory (DFT) calculations, element-specific X-ray spectroscopy techniques and in situ atomic force microscopy (AFM) to unravel the electronic ground structures and the oxidation states of the prototypical Mn-5,10,15-tris(pentafluorophenyl)corrole complexes as well as of their thermally induced derivatives adsorbed on Ag(111).

Our results, in particular the theory-assisted interpretation of Mn photoemission and absorption fine structure spectra, enable a comprehensive understanding and a deep insight into the on-surface chemistry of such complex molecular systems on the atomic-scale level.

O 44.6 Tue 18:00 Poster D

Changing the Characteristic Critical Current in an STM Josephson Junction by Magnetic Adatoms — •Rika Simon[1], Nils Bogdanoff[1], Olof Peters[1], Gaël Reecht[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Univ. Grenoble Alpes, Institut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

Atomic spins on superconducting surfaces introduce so called Yu-Shiba-Rusinov (YSR) states inside the superconducting gap as a fingerprint of magnetic interaction. Additionally, a renormalization of the local order parameter is predicted by theory, which is not directly reflected in the differential conductance spectra. In contrast, the order parameter can be determined directly in a Josephson junction by measuring its characteristic critical current. The use of a superconducting tip and substrate creates this SIS Josephson junction in a scanning tunneling microscope (STM). The atomic scale spatial resolution of the STM enables the measurement of the critical current on individual magnetic adatoms. A depletion in critical current can be observed on Fe adatoms on a Pb(110) surface [1].

Here, we present further work investigating the seemingly even greater changes in critical current caused by Mn adatoms on Pb(111) in voltage- and current-biased Josephson junctions.
[1] M. T. Randeria, B. E. Feldman, I. K. Drozdov, and A. Yazdani, Scanning Josephson spectroscopy on the atomic scale, Phys. Rev. B 93, 161115(R), 2016

O 44.7 Tue 18:00 Poster D

DFT calculation and experimental study on structural, optical and magnetic properties of Co-doped SrTiO3 — •Pornsawan Sikam[1], Pairot Moontragoon[1,2,3,4], Chayanin Sararat[1], Attaphol Karaphun[1], Ekaphan Swatsitang[1,2,3], Supree Pinitsoontorn[1,2,3], and Prasit Thongbai[1,2,3] — [1]Department of Physics, Khon Kaen University, Khon Kaen, 40002, Thailand — [2]Integrated Nanotechnology Research Center (INRC), Department of Physics, Khon Kaen University, Khon Kaen, 40002, Thailand — [3]Nanotec-KKU Center of Excellence on Advanced Nanomaterials for Energy Production and Storage, Khon Kaen University, Khon Kaen, 40002, Thailand — [4]Thailand Center of Excellence in Physics, Commission on Higher Education, Bangkok, 10400, Thailand

Outstanding features of SrTiO3 are thermal stability and photocorrosion resistance so the SrTiO3 is widely studied to apply as photocatalyst. However, for further applications, this work would like to study Co doping on the SrTiO3. It is questioned up whether d-orbital of Co could induce magnetism in the non-magnetic SrTiO3 or not because magnetism could improve applications of the SrTiO3. Here, the Co-doped SrTiO3 is studied both experimental and theoretical aspects. In experiment, the Co-doped SrTiO3 is prepared by hydrothermal method. From the experiment, it is seen that Co can improve not only magnetic and optical properties but also surface area of the SrTiO3. These observed results are corresponding to the DFT study. Therefore, it is possible that Co-doped STO might be a potential candidate to be a great photocatalyst and the diluted magnetic semiconductor.

O 45: Poster Tuesday: Ultrafast Processes

Time: Tuesday 18:00–20:00 Location: Poster D

O 45.1 Tue 18:00 Poster D

Four-dimensional XUV time- and angle-resolved photoemission spectroscopy of solids at 500 kHz — Michele Puppin[1,2], Christopher W. Nicholson[1,3], •Samuel Beaulieu[1], Shuo Dong[1], Tommaso Pincelli[1], Patrick Xian[1], Maciej Dendzik[1], Yoav W. Windsor[1], Yunpei Deng[1,4], Claude Monney[1,3], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]1Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin — [2]2Laboratory of Ultrafast Spectroscopy, ISIC, and Lausanne Centre for Ultrafast Science (LACUS), Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — [3]4Department of Physics, University of Fribourg, Chemin du Musee 3, 1700 Fribourg, Switzerland — [4]3Paul Scherrer Institute, Swiss FEL, 5232 Villigen PSI, Switzerland

We report on four-dimensional time- and angle-resolved photoelectron spectroscopy (trARPES) employing a 500 kHz extreme-ultraviolet (XUV) light source operating at 21.7 eV probe photon energy [1]. This beamline is coupled to a state-of-the-art time-of-flight momentum microscope (METIS 1000, SPECS GmbH) that allows us to measure the out-of-equilibrium multidimensional electronic band structure of solids (including excited states) in the entire Brillouin zone and with a temporal system response function below 40 fs. Exemplary data on inorganic and organic semiconductors will be presented. [1] Puppin et al., arXiv:1811.06939v1 [physics.ins-det] (2018).

O 45.2 Tue 18:00 Poster D

Multidimensional photoemission spectroscopy data: A framework for distributed and volumetric processing — Rui P. Xian[1], Yves Acremann[2], Steinn Y. Agustsson[3], Maciej Dendzik[1], Davide Curcio[4], Dmytro Kutnyakhov[5], Ralph Ernstorfer[1], and •Laurenz Rettig[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Department of Physics, ETH, Zurich, Switzerland — [3]Department of Physics, University of Mainz, Mainz, Germany — [4]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [5]DESY Photon Science, Hamburg, Germany

Recent developments of photoelectron spectrometers based on time-of-flight techniques using multi-dimensional delay-line detectors such as k-TOFs and momentum microscopes are fueling the emerging field of multidimensional photoemission spectroscopy (MPES). It enables a rapid volumetric mapping of the electronic band structure of materials and naturally incorporates further dimensions such as k_z dispersion, spin or pump-probe time. A significant challenge for the data handling are the high throughput data streams of individual detected electrons with multi-dimensional coordinates, and the vast amount of events needed to fill a typical dataset, which reach into the order of hundreds of millions to tens of billions and requires histogramming, corrections and calibrations to convert into a structured format. We have developed a distributed open-source pipeline to process these data streams for use at large facilities and in tabletop experiments. Event-wise operation allows reliable experimental diagnosis and artifact correction.

O 45.3 Tue 18:00 Poster D

Development of a sub 50 fs mid-infrared laser source using the principle of OPCPA — •Manuel Bridger, Oscar Naranjo, Alexander Tarasevitch, and Uwe Bovensiepen — Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, Germany

For many different experiments to measure the lattice modes or molecular vibrations, it is essential to have an ultrashort laser pulse with a wavelength which is in resonance with such processes, namely in the mid infrared (MIR) range. Additionally it has been shown that the cutoff frequency of high harmonics can be increased into the keV X-ray range using longer wavelengths, which will be our central application for the MIR light [1].

We will present the development of a high peak power two step Optical Parametric Chirped Pulse Amplifier (OPCPA). With this procedure, it is possible to switch the wavelength from the visible range towards the MIR by simultaneously increasing the pulse energy by several orders of magnitude.

We start out with a Ti:sapphire oscillator yielding an octave-spanning spectrum around 800 nm, which is first stretched from 6 fs to 6 ps. Within two subsequent steps consisting of amplification using an OPA stage and wavelength switching within a DFG stage, we reach 3200 nm central wavelength with a bandwidth supporting sub 50 fs and a pulse energy of >500 μJ. This work is funded by the DFG through SFB 1242, TP A05.

[1] T. Popmintchev et al., Science 336, 1287-1291 (2012).

O 45.4 Tue 18:00 Poster D

Analysis of the Excited State Potential Energy Surface of an Ultrafast Charge-Density-Wave-to-Metal Transition — •J. Maklar[1], W. Windsor[1], C. Nicholson[1], V. Esposito[2], P. Walmsley[3], M. Puppin[1], E. Bothschafter[2], M. Porer[2], J. Rittmann[2], D. Leuenberger[4], M. Kubli[5], M. Savoini[5], E. Abreu[5], S. Johnson[5], I. Fisher[3], P. Beaud[2], G. Ingold[2], U. Staub[2], R. Ernstorfer[1], M. Wolf[1], and L. Rettig[1] — [1]Fritz-Haber-Instiitut der Max-Planck-Gesellschaft, Berlin, Deutschland — [2]SLS, Paul Scherrer Institut, Villigen, Schweiz — [3]GLAM, Department of Applied Physics, Stanford, California, USA — [4]Department of Physics, Univ. Zürich, Schweiz — [5]Inst. für Quantenelektronik, ETH Zürich, Schweiz

Charge-density-waves (CDWs) exhibit a fascinating broken-symmetry ground state due to their intertwining with high-Tc superconductivity, their competition with Mott physics, and their interaction with magnetism. In this study we investigate the electronic and structural dynamics of the prototypical 2D CDW compound TbTe3 using XUV time-resolved ARPES and time-resolved X-ray diffraction. We observe a CDW-to-metal transition concomitant with a strongly fluence-dependent coherent oscillatory behavior of the electronic band gap and a simultaneous suppression of the periodic lattice distortion. Based on a Ginzburg-Landau-type approach we discuss how to extract the excited state energy potential of the order parameter and how to access the coupling strengths between different degrees of freedom on a quantitative level.

O 45.5 Tue 18:00 Poster D

High harmonic generation up to the keV regime and further applications of mid-infrared radiation — •Oscar Andres Naranjo Montoya, Manuel Bridger, Alexander Tarasevitch, and Uwe Bovensiepen — Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, Germany

Pump-probe experiments with optical excitation and absorption spectroscopy in the soft X-ray range on a femtosecond timescale are useful to analyze electronic and magnetic properties of complex material systems and their temporal evolution. Tabletop generation of soft x-rays pulses has become available using high harmonic generation driven by mid-infrared (MIR) femtosecond pulses in noble gases[1].

We developed a two-step Optical Parametric Chirped Pulse Amplifier that delivers sub 50 fs pulses at a wavelength of 3200 nm and energy $>500\ \mu$J as a pump for a tabletop soft x-ray source. That opens a door to perform a wide variety of soft x-ray experiments. Moreover, this MIR source also allows us to observe Floquet-Bloch states on the surfaces of topological insulators by femtosecond photoelectron spectroscopy[2]. We present the achieved spatial, spectral and temporal pulse characteristics of the MIR source as well as the estimate soft x-ray flux with some of the applications to be developed.

This work is funded by the DFG through SFB 1242, TP A05.

[1] T. Popmintchev et al., Science **336**, 1287 (2012).

[2] F. Mahmood et al., Nature Phys. **12**, 306 (2016)

O 45.6 Tue 18:00 Poster D

Development of time-resolved photoemission electron microscopy of magnetization dynamics triggered by back-side illumination — •Maximilian Paleschke, Cheng-Tien Chiang, and Wolf Widdra — Institute of Phyiscs, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany

Over the last decades, both ultrafast microscopy and spintronics have progressed in a remarkable manner. Experimental and theoretical methods have been developed in order to understand and control the spin transport and magnetization dynamics approaching the spatial-temporal limit of available techniques [1]. Supported by the newly founded CRC/TRR 227 Ultrafast Spin Dynamics we set up an experiment for spin and magnetization dynamics of magnetic thin films on nanometer-femtosecond scales. Our approach combines state-of-the-art time-resolved photoemission electron microscopy (PEEM) with a back-side pumping geometry. With this setup, we image magnetic domains using magnetic dichroism in photoemission [2] and record nm-fs movies of domain switching and domain wall motion triggered by fs spin and optical excitations. In this poster, we will present our experimental setup including quantitative estimations of the excitation density required to trigger ultrafast magnetization dynamics, the accessible temporal resolution, as well as the size of the magnetic linear and circular dichroic effects in PEEM.

[1] A. Kirilyuk et al., Rev. Mod. Phys. 82, 2731 (2010)

[2] C. M. Schneider, G. Schönhense, Rep. Prog. Phys. 65, 1785 (2002); W. Kuch, C. M. Schneider, ibid. 64, 147 (2001)

O 45.7 Tue 18:00 Poster D

Band Occupation and Optical Response of Gold far from Equilibrium — •Pascal D. Ndione[1], Sebastian T. Weber[1], Dirk O. Gericke[2], and Baerbel Rethfeld[1] — [1]Department of Physics and OPTIMAS Research Center, TU Kaiserslautern, Germany — [2]Centre for Fusion, Space and Astrophysics, Department of Physics, University of Warwick, UK

Short laser pulses drive materials into a nonequilibrium state. Then due to diverse scattering processes, a new thermodynamic equilibrium is reached. It is important to understand the transient changes of the optical properties which strongly depend on the nonequilibrium electrons dynamics within the bands.

This contribution investigates the band occupation and the optical properties in gold upon excitation with a short laser pulse. We propose two different models depending on the photon energy of the applied excitation. With optical pulses, only d and sp-band electrons can be excited and electrons might be promoted into states above Fermi energy. The subsequent dynamics are calculated in a two-band model. On the other hand, X-ray light allows accessing deeper bands like the f-shell. In that case, more kinetic processes are at play and more bands are needed. Our model with three active bands allows tracing the occupation numbers for VUV excitation. With the bands' occupation, we are able to calculate the transient optical properties and make a comparison to experimental data.

O 45.8 Tue 18:00 Poster D

Picosecond acoustic waves in laser-excited metal-semiconductor heterostructures studied by ultrafast X-ray diffraction — •Fabian Brinks[1], Mohammadmahdi Afshari[1], Philipp Krumey[1], Andrey Akimov[2], Dmitri Yakovlev[3], Manfred Bayer[3], and Klaus Sokolowski-Tinten[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Lotharstrasse 1, 47048 Duisburg, Germany — [2]School of Physics and Astronomy, University of Nottingham, NG7 2RD, UK — [3]Faculty of Physics, Technical University Dortmund, 44221 Dortmund, Germany

Absorption of ultrashort optical pulses in solids leads to a quasi-instantaneous increase of stress/pressure, which is subsequently released by acoustic strain waves traveling through the sample. We investigate the excitation and transient evolution of such coherent acoustic phonons in metal-semiconductor heterostructures composed of thin metal films (Ti, Cr, Al, Pt, Au, Pd) deposited on 100-oriented GaAs substrates by time-resolved X-ray diffraction using ultrashort X-ray pulses at 4.5 keV from a fs laser-plasma X-ray source. By probing the GaAs (400) Bragg reflection in an optical pump - X-ray probe scheme we are able to monitor the strain waves. To reveal the underlying physical processes we follow a combined approach. Direct reconstruction of the strain profile together with simulation of the elastic wave equation followed by dynamical diffraction calculations give a complementary view on the material-dependent evolution of stress/strain upon ultrafast excitation.

O 45.9 Tue 18:00 Poster D

Suspended 2D-materials as targets for ps-ion source — Tobias Foller, Alexander Breuers, •Leonard Christen, Matthias Herder, Anke Hierzenberger, Andreas Wucher, and Marika Schleberger — Faculty of Physics, University of Duisburg-Essen, Germany

For a high yield in transmission experiments and experiments involving broad probing beams large area ultrathin targets are required. CVD-grown 2D materials are a suitable starting material for this purpose allowing possible applications [1] and experimental approaches [2,3]. Therefore, we have inherited [4] and adapted a new technique to fabricate large area suspended 2D-membranes. We start off with CVD-grown 2D material. Protected by a thin poly(methyl methacrylate) (PMMA) film the heterostructure is then transferred to a perforated substrate. Using the solvent replacement technique [4] PMMA is gently removed.

The duration of a secondary electron pulse is a direct image of the parent picosecond ion pulse. For our ion source creating picosecond pulses it is thus important to know the secondary electron emission and radiation hardness of the targets under Ar+ ion-irradiation. We have developed an experimental setup to investigate these characteristics.

[1] Cohen-Tanugi et al., Nano Lett., 7 (2012) pp 3602-3608 [2] Kotakoski et al., Nat. Commun. 5 (2014) 3991 [3] Gruber et al, Nat. Commun. 7 (2016) 13948 [4] Chen et al., Nanoscale 8 (2016) pp 3555-3564

O 46: Poster Tuesday: Plasmonics and Nanooptics

Time: Tuesday 18:00–20:00 Location: Poster D

O 46.1 Tue 18:00 Poster D

Multi-color holographic metasurfaces — •Bernhard Reineke[1], Basudeb Sain[1], Lingling Huang[1,2], and Thomas Zentgraf[1] — [1]Universität Paderborn Department Physik, Warburger Str. 100, 33098 Paderborn — [2]Beijing Institute of Technology School of Optoelectronics, Side Rd of N. 3rd Ring Rd W, Haidian Qu, Beijing Shi, China

A phase only hologram is the recording of the phase distribution of an object. This phase distribution can be used to reconstruct an image of the encoded object. Several approaches exist to encode the phase information onto a physical hologram. One way is to use specially designed silicon nanophotonic metasurfaces. Here, we use a metasurface made of silicon nanostructures that are rotated against each other to encode a phase information. In most cases, there is a certain need to extend the principles of holographic metasurfaces to a multi wavelength regime. In our work, we demonstrate a holographic Metasurface that consists of different silicon nanostructures optimized for two different wavelengths in the visible spectral range. We show how this metasurface behaves in transmission, if it is illuminated with different wavelengths from a coherent light source. Furthermore, we retrieve a color image when the metasurface is illuminated with light of different wavelengths. Our approach opens new ways for improved multi-color anticounterfeit measures or new ways of color display systems.

O 46.2 Tue 18:00 Poster D

Accurate positioning of quantum dots by means of dielectrophoresis — •Patrick Pertsch[1], René Kullock[1], Monika Emmerling[1], Noga Meir[2], Dan Oron[2], and Bert Hecht[1] — [1]NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany — [2]Nanophotonics Laboratory, Weizmann Institute of Science, Israel

Semiconductor quantum dots (QDs) attract a lot of interest due to their tunable light emission, high efficiency and single-photon characteristics. Combining them with optical antennas can not only lead to strong coupling [1] but further enhance the emission and directionality of the radiation. To achieve that the QDs have to be positioned accurately which, in the past, has been realized by complex and time consuming processes [2,3].

Here we report on a much simpler process, utilizing dielectrophoresis, to load the gap of an electrically connected antenna with colloidal QDs. The dot-in-rod QDs align along the 30-nm gaps of the dimer antennas, show strong photoluminescence and are promising for electro-optical applications. This method is not restricted to the dimer antennas and allows accurate preparation of QD-antenna systems within a few minutes.

[1] H. Groß et al., Science Advances 4, eaar4906 (2018)
[2] A. G. Curto et al., Science 329, 930-933 (2010)
[3] E. Tranvouez et al., Nanotechnology 20, 165304 (2009)

O 46.3 Tue 18:00 Poster D

First steps towards strong coupling between emitters and plasmonic lattices — •Christoph Schnupfhagn, Simon Durst, Thorsten Schumacher, and Markus Lippitz — Experimental Physics III, University of Bayreuth, Germany

Plasmonic nanostructures allow to increase the interaction with light by resonant oscillations of the conduction electrons. When arranged in a lattice with a periodicity comparable to the optical wavelength, plasmonic nanoparticles can diffractively couple in the far-field, giving rise to surface lattice resonances. Consequently, the lattice structure generates a spatially extended mode while the plasmonic hotspots boost the light-matter interaction locally. It has already been shown that systems where emitters are coupled to these hybrid modes can serve as plasmonic nanolasers [1]. Furthermore, the small mode volume of the field hotspots allows to reach the strong coupling regime [2]. Here we present our first measurements on the dispersion relations of surface lattice resonances in gold nanoparticle arrays and their interaction with emitters.

[1] A. Yang et al., ACS Nano 2015, 9 (12), 11582-8
[2] L. Shi et al., Phys. Rev. Lett. 2014, 112 (15), 153002

O 46.4 Tue 18:00 Poster D

Enhanced Confinement of Surface Plasmon Polaritons on InAs with a High Index Medium — •Konstantin G. Wirth, Lena Jung, Yixi Zhou, Andreas F. Hessler, and Thomas Taubner — Institute of Physics (IA), RWTH Aachen

The semiconductor InAs offers promising properties for applications in the field of plasmonics due to its low damping and easy tunabilty compared to metals and other semiconductors. Recently, on InAs-Nanowires 1D surface plasmons (SP) with a high confinement of $\lambda_0/\lambda_p = 34$ and low damping rate have been observed by using infrared nearfield microscopy (s-SNOM)[1]. Simulations suggest that by depositing a thin layer of a high index material on the InAs an enhanced confinement of the SP can be achieved. In our work we use the phase change material (PCM) $Ge_3Sb_2Te_6$ as high index medium, which is switchable between an amorphous and a crystalline phase accompanied by a large refractive index change and low dielectric loss in the IR[2]. Switching the PCM between its amorphous and crystalline phase would further enable us to control the wavelength of the SP as well as its damping.

[1] Y. Zhou et al., Adv. Mater. 2018, 1802551
[2] A.-K. U. Michel et al., Adv. Optical Mater. 5, 1700261 (2017)

O 46.5 Tue 18:00 Poster D

Extracting the electronic properties of an oxide two-dimensional electron gas by scanning near-field optical microscopy — •Julian Barnett[1], Martin Lewin[1], Marc Rose[2], Felix Gunkel[2], Regina Dittmann[2], and Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen — [2]Peter Grünberg Institut, Forschungszentrum Jülich GmbH

In the family of functional oxide materials one interesting system is the interface between bulk insulators $SrTiO_3$ and $LaAlO_3$ (LAO/STO), which gives rise to a confined and highly conductive two-dimensional electron gas (2DEG) [1]. This 2DEG exhibits remarkable properties such as superconductivity and gate tunability, while displaying the possibility for future transistor applications. Infrared spectroscopy can be employed for the characterization of 2DEG structural and electronic properties, such as confinement dimensions, carrier density and mobility, but is diffraction-limited in its lateral resolution.

Here, scanning near-field optical microscopy (SNOM) is used to overcome this limitation and obtain nanoscale IR spectra of buried LAO/STO interfaces in the range of the near-field phonon resonance, as the local electronic properties of STO can be quantified by exploiting plasmon-phonon coupling [2]. We will investigate the impact of variations in local topography and interface termination on 2DEG formation to better understand the underlying principles and enable controlled manipulation of its electronic properties.

[1] A. Ohtomo et al., Nature 427, 423 (2004).
[2] M. Lewin et al., Adv. Funct. Mater. 28, 1802834 (2018).

O 46.6 Tue 18:00 Poster D

Localization of photonic modes in optimised disordered amorphous silicon thin films — •Felix Becker[2], Martin Aeschlimann[1], Tobias Brixner[3], Benjamin Frisch[1], Michael Hartelt[1], Matthias Hensen[3], Thomas H Loeber[4], Walter Pfeiffer[2], Sebastian Pres[3], Bernd Stannowski[5], and Helmut Stiebig[2] — [1]Fachbereich Physik and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern — [2]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld — [3]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [4]Nano-Structuring-Center, Erwin-Schrödinger-Str. 13, 67663 Kaiserslautern — [5]Helmholtz-Zentrum Berlin, PVcomB, Schwarzschildstr. 3, 12489 Berlin

Tailored disordered nanostructures that feature long-living photonic modes are employed to enhance local light scattering, light localization, and absorption. We demonstrate the controlled fabrication of nanotextured a-Si:H absorber layers using focused ion beam milling of planar ZnO_x substrates and PECVD. This allows studying the light absorption in nanotextured absorber layers with custom designed topographies. Light trapping and absorption in these samples is investigated by time- and energy-resolved PEEM. The obtained map of photonic modes and absorption patterns agrees well with FTDT simulations. We demonstrate enhanced light localization in tailored disordered absorbers and demonstrate a new strategy to further optimize light trapping.

O 46.7 Tue 18:00 Poster D

Femtosecond pulse compression for nonlinear spectroscopy — •Johannes Klier, Christoph Schnupfhagn, Julian Obermeier, and Markus Lippitz — Experimentalphysik III, University of Bayreuth, Germany

A pulse shaper makes it possible to manipulate arbitrarily the phase and amplitude of a femtosecond laser pulse. This is very useful for nonlinear spectroscopy since electric fields for multi-photon processes can be generated very accurately. Therefore, it is important that the pulse does not experience any broadening in time domain when coupled into a high-NA microscope. This compensation of the pulse chirp can be done with different nonlinear processes. Two photon absorbtion or the FWM-signal of samples with a large third-order nonlinear susceptibility $\chi^{(3)}$ in combination with phase-resolved interferometric spectral modulation (PRISM) are well suited for achieving this task. Here we present our experimental setup and results on pulse compression in the focal plane. Moreover, we give an overview how multi-photon excitation of dyes and graphene can be implemented in future experiments.

O 46.8 Tue 18:00 Poster D

Combining fluorescence and photoemission electron microscopy for the investigation of ultrafast surface phenomena — •Daniel Fersch[1], Sebastian Pres[1], Bernhard Huber[1], Victor Lisinetskii[1], Matthias Hensen[1], Enno Krauss[2], Bert Hecht[2], Heiko Lokstein[3], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]NanoOptics & Biophotonics Group, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Department of Chemical Physics and Optics, Charles University Prague, 121 16 Praha 2, Czech Republic

To learn something about individual quantum systems and their interaction with the environment it is advantageous to look beyond the optical diffraction limit on ultrashort timescales. For this purpose, we use a scanning fluorescence microscope as well as an aberration-corrected photoemission electron microscope combined with a NOPA-based laser source, giving us an effective temporal and spatial resolution of sub-20 fs and sub-10 nm, respectively. Here, we present results on the polarization-dependent fluorescence enhancement of cyanobacterial Photosystem I thin films by gold nanorods, as well as first photoemission images of the protein dropcasted on monocrystalline gold flakes. We further show fluorescence and time-resolved photoemission from low-dimensional nanostructures performed with our pulse shaper. Finally, we want to use our microscopes to compare fluorescence-based multidimensional spectroscopy and coherent two-dimensional nanoscopy on the same samples.

O 47: Poster Tuesday: Scanning Probe Techniques

Time: Tuesday 18:00–20:00 Location: Poster D

O 47.1 Tue 18:00 Poster D

Simulation of STM images and spectroscopy of single nitrogen-doped molecules with 5-7 membered rings on Au(111) surfaces — •Seddigheh Nikipar[1,3,4], Dmitry A. Ryndyk[1,2], Sibylle Gemming[3,4], Francesca Moresco[1,4], Gianaurelio Cuniberti[1,4], and Thomas Frauenheim[2] — [1]Institute for Materials Science, TU Dresden — [2]BCCMS, Department of Physics, Universität Bremen — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — [4]Center for Advancing Electronics Dresden, TU Dresden

We consider STM images and spectroscopy (STS) of molecules on metal surfaces. We combine DFT based atomistic tight-binding model (DFTB approach) with Green function technique, which offers a framework to consider tip, molecule and surface as one integrated system and taking into account the tip geometry. Besides, it captures the interference and interaction effects. This approach can be applied for the investigation of finite-voltage effects and describe the high-energy molecular transport states. It allows to simulate quantitatively the I(V) current-voltage spectroscopy curves and dI/dV maps in both constant current and constant height modes. We applied our methods to nitrogen-doped molecules with 5-7 membered rings on Au(111) surface and showed that the electronic properties of molecules are strongly influenced by formation of azulene-motifs. We developed the integrated open software suite for quantum nanoscale modeling (TraNaS OpenSuite, tranas.org/opensuite) for convenient calculations of large-scale molecular nanosystems on metal surfaces.

O 47.2 Tue 18:00 Poster D

Nano-manipulation on the polymer surfaces using functionalized AFM probes — •Tunç Çiftçi[1], Laurent Pham Van[2], Oleg Kurnosikov[1], and Bert Koopmans[1] — [1]Eindhoven University of Technology, Eindhoven, the Netherlands — [2]Centre CEA de Saclay, Gif-sur-Yvette, France

We demonstrate a new approach to manipulate various polymer surfaces by an AFM using specifically designed probes. By this new method, the submicrometer protrusions can be formed on the surface in any selected positions. In contrast to the earlier approaches based on deforming thick organic materials by pressing with a probe, we form protrusions without any tip-surface contact. These functionalized probes can generate an instant temperature gradient at the tip while remaining in the non-contact regime close the surface. The high temperature gradient at the tip end can be switched on and off sharply. The organic material is heated up to its melting point quickly and locally pulled up towards to the hot tip by the van der Waals forces. With a sharp drop in the temperature, this fluidic-protrusion solidifies maintaining its shape. To realize this functionality, we implemented a new type of conducting planar probes, which provide high current density close to the tip end for controlling the local temperature. With this design we can manipulate a broad class of organic materials with melting temperature from 20 up to 400 degrees of Celsius. Our approach is also could be challenging for study and selective manipulation of biological systems.

O 47.3 Tue 18:00 Poster D

High resolution imaging of organic molecules using Q-controlled amplitude modulation atomic force microscopy with CO-functionalized tips — •Daniel Martin-Jimenez[1], Alexander Ihle[1], Sebastian Ahles[2], Hermann A. Wegner[2], Andre Schirmeisen[1], and Daniel Ebeling[1] — [1]Institute of Applied Physics (IAP), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Institute of Organic Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany

The so-called bond imaging atomic force microscopy (AFM) technique has become an invaluable tool for studying organic molecules on surfaces. The key feature of this technique is to functionalize the AFM-tip with a single molecule, e.g., CO. Hereby, the imaging capabilities of dynamic mode AFM are improved, which allows to determine the precise orientation and internal structure of adsorbed organic molecules. Usually, these measurements are performed by operating tuning fork sensors in frequency modulation mode at low temperatures in ultrahigh vacuum conditions. The high quality factors of the tuning fork sensors under these conditions typically prohibit operation in amplitude modulation mode due to the slow response time caused by the low damping environment. Here, we use the Q-control technique to reduce the effective quality factor of the sensor from about 30000 to 3000. This enables submolecular amplitude modulation imaging with a lateral resolution and signal to noise performance comparable to frequency modulation mode.

O 47.4 Tue 18:00 Poster D

Quantitative Kelvin probe force microscopy on nanoscale devices — Amelie Axt[1], Ilka M Hermes[1], Rüdiger Berger[1], and •Stefan A.L. Weber[1,2] — [1]MPI for Polymer Research Mainz, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, Germany

We investigate the influence of the operation method in Kelvin probe force microscopy (KPFM) on the measured potential distribution. KPFM is widely used to map the nanoscale potential distribution in operating devices, e.g. in thin film transistors or on cross sections of functional solar cells [1]. Quantitative surface potential measurements are crucial for understanding the operation principles of functional nanostructures in these electronic devices. Nevertheless, KPFM is prone to certain imaging artifacts, such as crosstalk from topography or stray electric fields. Here, we compare different Amplitude Modulation (AM) and Frequency Modulation (FM) KPFM methods on a reference structure with a defined potential difference [2]. In particular, we investigate how quantitative the externally applied voltage is measured. We found that even in the presence of a strong stray field, the FM KPFM methods measured more than 95% of the external bias, whereas the commonly used lift-mode AM KPFM measured less than 70% of the external bias. [1] Energy Environ. Sci., 2018,11, 2404; J. Phys. Chem. Lett., 2018, 9, 6249. [2] Beilstein J. Nanotechnol. 2018, 9, 1809.

O 47.5 Tue 18:00 Poster D

Optimization of the energy resolution and RF capability of a 30 mK dilution refrigerator scanning tunneling microscope — •Manuel Steinbrecher[1], Henning von Allwörden[1], Andreas Eich[1], Jan Gerritsen[1], Fabian D. Natterer[2], Daniel Wegner[1], and Alexander A. Khajetoorians[1] — [1]IMM, Radboud University Nijmegen, The Netherlands — [2]University of Zurich, Switzerland

For a scanning tunneling microscope (STM) operated with a metallic tip the energy resolution of the spectroscopic measurements typically is given by the effective temperature of the tunneling electrons, namely $3.5k_\mathrm{B}T$. However, for temperatures below $\approx 100\,\mathrm{mK}$, contributions like the electromagnetic noise inside the system and capacitive noise become more dominant [1-2].

We use a home-made dilution refrigerator ($T = 30\,\mathrm{mK}$) based STM [3], with a vector magnet established in Nijmegen to test the energy resolution of our setup. We report on superconducting measurements of Al-Al junctions. We perform measurements in different tunneling regimes and with a variety of tips, testing both tip diameters and materials and report on their significance. In this course, the system was upgraded to RF capability for electron spin resonance (ESR) experiments [4]. Results and performance will be shown for a dilution fridge STM for the first time.

[1]D. Vion *et al.*,JoAP **77**, 2519 (1995)

[2] C. R. Ast *et al.*, Nat. Commun. **7**:13009 (2016)

[3] H. v. Allwörden *et al.*, RSI **89**, 033902 (2018)

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

O 47.6 Tue 18:00 Poster D

Automated Laboratory Monitoring based on the Internet of Things — •Nicolaj Betz[1], Max Hänze[1,2,3], Luigi Malavolti[1,2,3], Gregory McMurtrie[1,2,3], and Sebastian Loth[1,2,3] — [1]University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany — [3]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Precise environment control is a crucial factor for reliable scanning tunneling microscopy. The Internet of things is a network of devices and appliances that combine measurement and control features with a connectivity framework, thereby introducing the possibility of remotely monitor and control laboratory setups [1]. Here we present an implementation that is based on battery-powered microcontrollers and Wifi connectivity to enable the use of conventional lab equipment in a cloud-based measurement system. Our approach enables precise process monitoring and control of a sub-Kelvin high magnetic field scanning tunneling microscopy laboratory with a small budget.

[1] Jeffrey M. Perkel, Nature 542, 125 (2017).

O 47.7 Tue 18:00 Poster D

Modelling Photo-Assisted Scanning Tunneling Microscopy — •Ole Bunjes, Benjamin Schröder, Lara Wimmer, Claus Ropers, and Martin Wenderoth — Georg-August-Universität, IV. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen

Scanning Tunneling Microscopy (STM) offers unique capabilities in imaging and spectroscopy on the atomic scale. A promising approach to observe surface dynamics faster than electronic sampling speeds is the combination of STM with pulsed laser excitation.

Typically, the tunnel current $I(z)$ depends mono-exponentially on the tip-sample distance z. In recent experiments, we found a strong deviation from this typical exponential decay upon femtosecond laser illumination of the tunnel junction.

We explain this observation by modelling the vacuum barrier including a one-dimensional image potential and an effective electron energy distribution. We simulate the energy-, distance- and bias-voltage-dependent transmission probabilities. In combination with a series of fermionic distributions of different amplitudes, temperatures and energy intervals, we model the measured $I(z)$ curves. This approach allows us to quantify the contributions of hot electrons as well as multi-photon excited electrons to the tunneling current. We provide a comprehensive picture including voltage- and laser-power-dependent data.

This project is financially supported by the DFG in the SFB 1073 (project C4).

O 47.8 Tue 18:00 Poster D

Atomic Manipulation in NC-AFM Experiments: The Influence of the Chemical Tip Termination — •Damla Yesilpinar, Alexander Timmer, Bertram Schulze Lammers, Harald Fuchs, and Harry Mönig — Physikalisches Institut, WestfälischeWilhelms-Universität Münster

Controlled manipulation of atoms and molecules on the surface by an NC-AFM tip allows measuring the forces during the manipulation. The underlying mechanism has previously been attributed to lowering of the diffusion barrier due to the interaction between the tip and the manipulated particle. In this study, we have examined the effect of different chemical tip terminations on the manipulation processes. As a model system, we have chosen Xe atoms on a partially oxidized Cu(110) surface. This surface exhibits the typical p(2x1)O-reconstructed oxide stripes alternating with pure Cu domains. STM images showed that Xe atoms were preferentially adsorbed at the metal/metal-oxide boundaries. The manipulation experiments were carried out along and perpendicular to the oxide rows with metallic-, Xe-terminated and CuOx-functionalized [1] tips. While each tip was able to manipulate the Xe atoms along the oxide row, only CuOx tips allowed successful manipulations above the pure Cu domains. This work sheds light on the pronounced influence of the chemical tip termination in such experiments and provides insights on the mechanisms of the preferential adsorption at the metal/metal-oxide boundaries [2]. [1]ACS Nano 2016, 10, 1, 1201-1209 [2]Nano Lett. 2018, 18, 7, 4123-4129

O 47.9 Tue 18:00 Poster D

dS11/dV spectroscopy and imaging of buried nanostructures — •Alexander Kölker[1,3], Georg Gramse[2,4], Matthias Koch[3], Ferry Kienberger[4], and Neil Curson[1] — [1]London Centre of Nanotechnology, UCL, London, UK — [2]Johannes Kepler University, Biophysics Institute, Linz, Austria — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [4]Keysight Laboratories, Keysight Technologies, Inc.,Linz, Austria

Non-destructive device characterization is especially of interest when including newly emerging materials like δ-layers, nanowires, graphene or spintronics in the fabrication processes. Scanning microwave microscopy (SMM) is a non-destructive technique that allows advanced characterization of electrical properties, such as carrier concentration, capacitance and conductivity, by measuring the reflected signal power (S11) of an electro magnetic wave guided to the AFM tip [1].

Further information, such as capacitance and conductance derivative (dC/dV and dG/dV) can be extracted by exploiting the field effect of a DC bias, applied in addition to the low RF signal to the tip.

Here we demonstrate for buried δ-layer nanostructures how dS11/dV spectroscopy in conjunction with FEM-modelling can be employed to identify contributions to the admittance that originate from the substrate, the patterned δ-layer region and its 2D nature. In the outlook we report on the development of a novel SPM sample that hosts an integrated circuit for in-situ single-molecule charge transport measurements. [1] G. Gramse, A. Kölker et al. Science Advances, vol. 3, no. 6, p. e1602586, 2017.

O 47.10 Tue 18:00 Poster D

A cryogen-free low-temperature scanning tunneling microscope — •Lukas Arnhold[1], Gregory McMurtrie[1], Stephan Spieker[1], Luigi Malavolti[1,2], and Sebastian Loth[1] — [1]Universität Stuttgart — [2]Max-Planck-Institut für Festkörperforschung

State of the art Scanning Tunneling Microscopes (STM) are inherently limited in their continuous measurement time by their cryocooling systems, making the acquisition of high resolution differential conductivity maps and other time consuming experiments challenging.

Gifford-McMahom (GM) cryocoolers [1] feature an extremely long hold time [2], but tend to introduce a degree of vibration which aggravates their use in scanning probe techniques.

In this homebuilt STM, we decouple a GM crycooler from the microscope head using a two-frame support system.

Performance tests indicate sufficient vibration suppression to perform high-quality STM measurements that can last as long as the cryocooler can operate.

Such extended hold-time STM's open the possiblity of investigating novel surfaces with unprecedented resolution and extended parameter spaces.

[1] J. Hacklez, High-stability cryogenic scanning tunneling microscope based on a closed-cycle cryostat, Review of Scientific Instruments 85, 103704 (2014) [2] S. Zhang, A cryogen-free low temperature scanning tunneling microscope capable of inelastic electron tunneling spectroscopy, Review of Scientific Instruments 87, 063701 (2016)

O 47.11 Tue 18:00 Poster D

Temperature dependence of directional nanofriction on NaCl — •Jennifer Konrad, Dirk Dietzel, and Andre Schirmeisen — Institute of Applied Physics, Justus-Liebig University Giessen, 35392 Giessen, Germany

On the nanometer scale, the directional dependence of friction is a well known phenomenon [1] that is typically related to the lattice structure of the sample with different energy barrier heights related to different sliding directions. Consequently, temperature should influence the friction pattern with more defined structures expected at low temperatures according to the concept of thermally activated friction. In this work, this fundamental assumption is analyzed by temperature dependent friction force microscopy on NaCl under UHV conditions. As a result, our measurements do not only document the general effect of temperature, but also highlight the additional influences of parameters like wear and tip shape on the effective friction pattern.

[1] S. G. Balakrishna, A. S. de Wijn, and R. Bennewitz, Physical Review B 89, (2014).

O 47.12 Tue 18:00 Poster D

Three dimensional tracing of the trajectory of a charged particle by electrostatic detection — •Erdem Genc, Doris Tarasevitch, Tobias Roos, Detlef Utzat, Hermann Nienhaus, and Rolf Möller — Fakultät für Physik/Cenide, Universität Duisburg-Essen, Germany

The position of a moving charged particle in free space is determined by using a configuration of electrodes in a parallel plate capacitor geometry. The electrodes are connected to ultra-sensitive and fast charge amplifiers [1] which measure the time-dependent displaced charge in the electrodes. In the experiment we trace the trajectory of a steel sphere of 1mm in diameter which falls freely and bounces off a surface. The initial charge on the sphere is 0.1pC. A spatial resolution of approximately 0.1mm perpendicular and 1mm parallel to the electrodes is achieved combined with a temporal resolution of better than 10 microseconds. In addition, the transfer of electric charge between the sphere and the electrodes during contact is evalutated for every collision. The experimental results are in excellent agreement with calculations applying classical electrodynamics. The method allows the access to charge transfer processes between colliding particles which is of high relevance in technology and fundamental research. [1] P. Graf. et al., Rev. Sci. Instrum. 88, 084702 (2017).

O 47.13 Tue 18:00 Poster D

Space and time-resolved unidirectional switching of single molecules — •Thomas Buchner, Dominik Peller, Lukas Kastner, Rupert Huber, and Jascha Repp — Department of Physics, University of Regensburg, 93040 Regensburg, Germany

Combining low-temperature scanning tunneling microscopy (STM) and ultrafast lightwave electronics has paved the way for tracking single molecule dynamics with combined atomic resolution and femtosecond temporal precision [1]. Here, we introduce single-shot detection in lightwave STM with single-electron control, opening the door to path-selective studies of unidirectional quantum events. We examine a magnesium phthalocyanine molecule, which adsorbs on sodium chloride in a bistable geometry. By means of single light pulses, single electrons can be deliberately injected into an unoccupied orbital, triggering the molecule to rearrange on the surface, eventually leading to a switching of its adsorption geometry. Monitoring a non-resonant cotunneling current allows one to detect every single switching event. In pump-probe experiments, the quantum yield for switching is measured for various parameters with combined sub-Å spatial and femtosecond temporal precision, which exhibits a distinct behavior for each reaction path. These multi-dimensional experimental data show marked oscillations in time and provide a fingerprint of the atomistic details of the molecular dynamics, at the sub-picosecond time scale.

[1] T. L. Cocker, D. Peller et al., Nature 539, 263-267 (2016)

O 48: Overview Talk: Henrik Grönbeck

Time: Wednesday 9:30–10:15 Location: H15

Invited Talk O 48.1 Wed 9:30 H15

Catalytic activity from first principles - towards operando computational catalysis — •Henrik Grönbeck — Chalmers University of Technology, Göteborg, Sweden

A key focus in heterogeneous catalysis is to understand the dominant reaction paths and isolate the character of the active sites. This is a challenge because of the dynamic character of the catalyst, which may undergo structural and phase changes as a response to the reaction conditions. To obtain information on the active site, the catalyst should preferably be characterized during operando conditions. The need to account for reaction conditions holds also computational work with the purpose to establish links between elementary steps and catalyst activity.

In this presentation, I will discuss our recent efforts to understand CO and methane oxidation over palladium and platinum using first principles calculations [1-5] exemplifying different aspects of operando computational catalysis. Special attention will be given our attempt to perform explicit simulations of reaction kinetics over metal nanoparticles. The examples will cover how composition, size, shape and strain may affect the catalytic turn over frequency.

[1] M. Jørgensen, H. Grönbeck, ACS Catalysis 6, 6730 (2016). [2] M. Van den Bossche and H. Grönbeck, J. Am. Chem. Soc. 137, 12035 (2015). [3] M. Jørgensen, H. Grönbeck, ACS Catalysis 7, 5054 (2017). [4] M. Jørgensen, H. Grönbeck, Angew. Chem. Int Ed. 57, 5086 (2018). [5] T. Nilsson Pingel, M. Jørgensen, A. Yankovich, H. Grönbeck, and E. Olsson, Nature Comm. 9, 2722 (2018).

O 49: Metal Substrates III: Structure, Epitaxy and Growth

Time: Wednesday 10:30–12:30 Location: H5

O 49.1 Wed 10:30 H5

Internal space analysis of a dodecagonal oxide quasicrystal and its approximants — •Sebastian Schenk[1], Stefan Förster[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

Two-dimensional oxide quasicrystals (OQC) with 12-fold symmetry have recently been derived from ultrathin perovskites on Pt(111) substrates [1,2]. They exhibit a tiling generated from quadratic, triangular, and rhombic elements of equal side length. By lifting the atomic coordinates of the tiling to a four-dimensional hyperspace, the structural properties of these monolayer structures are fully captured. The projection of the four-dimensional coordinates onto the so-called internal space allows a detailed analysis of the long-range ordering of the quasicrystal and a more precise differentiation between quasicrystals and their periodic approximant structures. Two different measures for the strength of the approximant structures will be given. As a tool for distinguishing defective quasicrystals from complex large unit cell periodic structures, the point distribution in the internal space and the phason strain matrix are discussed.
[1] S. Förster et. al., Nature **502**, 215 (2013)
[2] S. Schenk et. al., J. Phys.: Condens. Matter **29**, 134002 (2017)

O 49.2 Wed 10:45 H5

Electronic structure and property of ZnO/Ag(111): A combined study of UPS, LEED and STM — •Ting-Chieh Hung and Karina Morgenstern — Chair of Physical Chemistry I, Ruhr-University of Bochum, Germany

Zinc Oxide (ZnO) is a broad bandgap semiconductor, which is widely used as a catalyst. Therefore, the properties of ZnO have been investigated extensively. However, the microscopic views and properties of ZnO ultrathin film supported by metal single crystal have remained unexplored. We investigate the shifting and broadening of the surface state of Ag(111) with increasing ZnO coverage by ultraviolet spectroscopy (UPS). The UPS surface state results reveal an increasing intensity of the ZnO peak with increasing ZnO coverages, while the intensity of the Ag peak decreases. The low energy electronic diffraction (LEED) pattern shows the orientation of ZnO(0001) on Ag(111) with a lattice constant of (335±1) pm. We also confirmed the Moiré pattern of ZnO(0001) on Ag(111) [1] by our room temperature scanning tunneling microscopy (STM). Further STM results will be presented in this talk.

[1] Q. Pan et al, Catalysis Letters, 2014, 144(4), 648-655.

O 49.3 Wed 11:00 H5

Structure analysis of ultrathin NaCl-layers on various metallic substrates — •Kira Kolpatzeck, Ebru Ekici, Vijaya Begum, Markus Gruner, Rossitza Pentcheva, and Rolf Möller — Faculty of Physics and Center of Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

The electronic decoupling of single atoms, molecules or clusters from a metallic substrate gains in importance whenever radiative transitions shall be observed. Moreover, for various surface science methods, such as scanning tunneling microscopy, a non-vanishing surface conductivity is necessary. To combine those two requirements ultrathin insulating layers come into play. We have studied the growth of ultrathin NaCl films with various thicknesses on several copper and gold substrates by low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) at low temperatures (8 K and 80 K). As well-known from literature [1] the evaporation of NaCl onto a clean Cu(111) surface at room temperature leads to the growth of rectangular monolayer NaCl islands on top of a continuous NaCl film, which covers the surface partially. If the NaCl is deposited onto the heated copper surface, the formation of nanowires associated with dislocation lines is observed in our measurements. The study of evaporated NaCl on Au(110) also reveals two distinguishable superstructures, resulting from different arrangements of the interface atoms.

[1] R. Bennewitz, et al., Surf. Sci. 438, 289 (1999).

O 49.4 Wed 11:15 H5

Helical interdigitation of alpha-L polyalanine investigated by ambient STM — •Nguyen Thi Ngoc Ha[1], Yossil Patilte[2], and Christoph Tegenkamp[1,3] — [1]Technische Universitaet Chemnitz — [2]Department of Applied Physics, Hebrew University of Jerusalem, Israely — [3]Leibniz Universitaet Hannover, Germany

Polyalanine (PA) has an alpha-helix conformation, which is maintained by hydrogen bonds formed by backbone N-H and C=O groups of the amino acid located three or four residues earlier along the protein sequence. PA has gathered recently a lot of interest as the propagation of electrons along the helical backbone structure comes along with spin polarization of the transmitted electron. Self-assembly of PA molecules on HOPG substrate form two types of hexagonal structures: after showing a hexagonal structure with a next-neighbor distance of around 2.0nm, finally a well-ordered structure with closer lattice parameter (1.2nm) is found. This closed package structure is formed by the interdigitating between adjacent PA molecules due to the formation of additional hydrogen bonds from their helical back-bones and can be kinetically controlled by increasing the deposition tem- perature. The ordering within helical film refers to new ordering mechanism and can most likely explain the coherence in the electronic transport and high efficiency for the current induced spin selectivity[1] [1] R. Naaman, D. H. Waldeck, Annu. Rev. Phys. Chem. 66, 263-81, 2015.

O 49.5 Wed 11:30 H5

Formation of PtRu surface alloy on Ru(0001) substrate: A kinetic Monte Carlo study — •David Mahlberg and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Deutschland

Optimising the reactivity and selectivity of a specific catalytic reaction by the rational design of heterogeneous catalysts requires a comprehensive understanding of the factors underlying their reactivity and stability. A precise control of surface properties then allows to improve the performance of catalysts. In particular bimetallic surfaces offer the possibility to tailor their catalytic properties by deliberately modifying their composition and/or structural arrangement, which depends on the mixing ratio of the two metal elements.

We have studied the stability of PtRu/Ru(0001) surface alloys by kinetic Monte Carlo simulation using first-principles electronic structure calculations in order to derive the barriers for vacancy diffusion. Thus the structure formation of surface alloys on macroscopic time scales and mesoscopic length scales as a function of composition and temperature can be monitored for varying Pt concentrations. We will analyse the dependence of the diffusion barriers on the particular arrangement of the surface alloy based on the interaction between the constituents.

O 49.6 Wed 11:45 H5

Unexpected surface structure of the Rashba system Te/Ag(111) — •Tilman Kisslinger[1], Maximilian Ünzelmann[2], Hendrik Bentmann[2], Friedrich Reinert[2], Thomas Fauster[1], Alexander Schneider[1], and Lutz Hammer[1] — [1]Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Lehrstuhl für Experimentelle Physik VII, Julius-Maximilians Universität Würzburg

Materials with Rashba-split bands are of interest for the use in spintronics and are intensively studied by experiment and theory [1].
Especially the systems prepared by depositing one third of a monolayer of Pb, Bi, Te or Sb on Ag(111) and Cu(111), which are considered to be substitutional surface alloys, show a Rashba splitting for which the strength strongly depends on the outward relaxation of the guest atoms [2]. However, for the Te/Ag(111) system the Ag_2Te surface alloy structure was never proven so far.
Upon deposition of 0.33 ML of Te on Ag(111) at temperatures between 90 K and 1000 K (and annealing to at least 373 K) we observe the formation of a $(\sqrt{3}\times\sqrt{3})$R30°-structure. STM measurements reveal a perfectly ordered surface phase with terraces of the width of several thousands of Angströms. Our quantitative LEED-I(V)-analysis shows that the surface is a TeAg honeycomb layer, where the atoms occupy hcp sites of the Ag(111) substrate. This finding is supported by atomically resolved STM measurements and DFT simulations.
[1] G. Bihlmayer et al., New J. Phys. **17** 050202 (2015)
[2] Gierz et al., Phys. Rev. B **81**, 245430 (2010)

O 49.7 Wed 12:00 H5

Revisiting the O/Cu(111) system (again): Looking through the lens of theoretical surface spectroscopy and microscopy — •Taehun Lee[1], Yun-Jae Lee[1], Giyeok Lee[1], Krisztián Palotás[2], and Aloysius Soon[1] — [1]Department of Materials Science & Engineering, Yonsei University, Seoul 03722, Korea — [2]Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary

Oxidation of copper surfaces has been investigated for decades with the goal of understanding the rich surface phase space where oxygen interacts readily with copper under reactive conditions. Nevertheless, a systematic and thorough characterization of metal-supported Cu surface oxides is currently far from complete due to their structural complexity and sensitivity to the growth conditions. Here, we survey and study the various possible ultrathin oxidic structures of Cu using first-principles density-functional theory (DFT) calculations. Namely, we report the DFT-derived surface core-level shifts (CLS) and simulated scanning tunneling microscopy (STM) images (where the orbitals of the STM tip are explicitly considered) for various oxidic O/Cu structures, as well as those containing surface defects. Here, we provide a first-principles microscopic picture of the O/Cu(111) system to interpret and explain the structural ambiguities reported in recent CLS and STM experiments.

O 49.8 Wed 12:15 H5

Electronic and atomic structure of Bi(111) and anomalous behaviour after ion bombardment — •Kuanysh Zhussupbekov[1], Brian Walls[1], Andrey Ionov[1,2], Sergey Bozhko[1,2], Rais Mozhchil[2], Killian Walshe[1], and Igor Shvets[1] — [1]School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia

Defects in a surface crystal structure of layered materials lead to a local break of surface translational symmetry and can modify the surface states. In this work, Bi(111) surfaces cleaved at low temperature and ion etched are investigated by Low-Energy Electron Diffraction (LEED), X-ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS), Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) techniques. STM measurements on the Bi(111) crystal demonstrated different heights of the steps (mono- and bi-layered steps). Furthermore, STS revealed that these steps have slightly different electronic properties, likely correlated to the cleavage breaking covalent (mono-layer) vs Van der Waals (bi-layer) bonds. The Bi(111) surface after ion etching at 110 K and room temperature reveals anomalous behaviour of the surface crystal structure: it results in the formation of flat mono- and bi-layer terraces and surface periodicity as observed by LEED even after continuous ion sputtering. Analysis of the electronic density of states near the Fermi level measured by UPS did not observe a noticeable difference at the Fermi edge.

O 50: Plasmonics & Nanooptics III: STM and Time-Resolved Methods (joint session O/CPP)

Time: Wednesday 10:30–13:15 Location: H8

O 50.1 Wed 10:30 H8

Plasmon-assisted resonant electron tunneling in a scanning tunneling microscope junction — Shuyi Liu[1], Martin Wolf[1], and •Takashi Kumagai[1,2] — [1]Fritz-Haber Institute of the Max-Planck Society — [2]JST-PRESTO

Plasmon-induced phenomena have attracted increasing attention due to diverse applications in nanoscale science and technology [1]. Plasmonic nanocavities play a particularly important role because of their ability to confine light to nanometric volumes and generate a strong field enhancement. We report plasmon-assisted resonant electron tunneling from an Ag or Au tip to field emission resonances (FERs) of a Ag(111) surface induced by CW laser excitation of a scanning tunneling microscope (STM) junction at visible wavelengths [2]. As a hallmark of the plasmon-assisted resonant tunneling, we observe a downshift of the first peak in the FER spectra by a fixed amount equal to the incident photon energy. STM-induced luminescence measurement for the Ag and Au tip reveals the clear correlation between the laser-induced change in the FER spectra and the plasmonic properties of the junction. Our results clarify a novel resonant electron transfer mechanism in a plasmonic nanocavity. References: [1] M. L. Brongersma, N. J. Halas, P. Nordlander, Plasmon-induced hot carrier science and technology. Nat. Nanotechnol. 10, 25-34 (2015). [2] S. Liu, M. Wolf, T. Kumagai, Phys. Rev. Lett. in print, 10.1103/PhysRevLett.121.226802.

O 50.2 Wed 10:45 H8

Investigation of plasmon assisted light emission from heteroepitaxial system of Co islands on Cu(111) by scanning tunneling microscopy — •Vibhuti Rai[1], Kevin Edelmann[1,2], Lars Wilmes[1], Lukas Gerhard[1], and Wulf Wulfhekel[1,2] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie, 76344 Eggenstein-Leopoldshafen, Germany — [2]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Scanning tunneling microscopy (STM) with optical access allows systematic and controlled investigation of light emission from nanometer-sized structures[1]. Here, plasmon mediated light emission from a heteroepitaxial system of bilayer and trilayer Co islands on Cu(111) is studied in ultra-high vacuum at low temperature (4.4 K). Electrical spectroscopy and optical spectroscopy were performed on an image size of 40 x 40 nm where an optical spectrum was taken at every point of a 160 x 160 grid. These measurements show the effect of geometric cavity alteration and the associated resonance shift, influence of dielectric constant of the sample and the tip, and modulation of emission intensity by Friedel oscillation. Interestingly, the results indicate that the difference in the yield of inelastic tunneling dominates over the difference of the gap plasmon resonance.

[1] K. Edelmann et al. Rev. Sci. Instrum. accepted for publication.

O 50.3 Wed 11:00 H8

Photon super-bunching from a metal-metal tunnel junction — Christopher C. Leon[1], Anna Rosławska[1], •Abhishek Grewal[1], Olle Gunnarsson[1], Klaus Kuhnke[1], and Klaus Kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale de Lausanne, Switzerland

Generating correlated photon pairs at the nanoscale is a prerequisite to creating highly-integrated optoelectronic circuits that perform quantum computing tasks based on heralded single-photons. Here, we report on the observation of bunched light emission from a generic tunnel junction under DC-bias. Using LT-STM coupled with Hanbury Brown-Twiss interferometer we probe the dynamics of the photon stream emitted by a metal-metal junction. The inelastic tunneling events of single electrons produce a plasmonic emission whose bunching factor can be 17 (super-bunching) when measured with 53 picosecond instrument resolution. Spectral filtering indicates that two photons of energy higher and lower than half the tunneling electron energy participate in bunching.

We show that mechanisms such as mechanical instabilities at the tip apex, electron co-tunneling, and electronic detection artifacts can be excluded, confirming the non-triviality of the emission. The $1e^- \rightarrow n\gamma$ process is promoted by the localized Purcell effect in conjunction with optical nonlinearities due to inversion symmetry breaking at the tunnel junction. The results suggest that an optoelectronic component useful for quantum computing can be miniaturized to the atomic scale.

O 50.4 Wed 11:15 H8

Simulating ultrashort light pulses in STM tunnel junctions — •Alexander Neef[1], Dominik Peller[2], Rupert Huber[2], and Jascha Repp[2] — [1]Fritz-Haber-Institute of the MPG, D-14195, Berlin,Germany — [2]Fakultaet fuer Physik, Universitaet Regensburg, D-93040 Regensburg, Germany

Combining ultrafast lightwave control and scanning tunneling miscroscopy (STM) recently opened the door to atomic-scale femtosecond imaging [1,2]. In lightwave STM, a THz field transient is coupled into the tunneling junction to apply an ultrashort bias voltage. The near-field waveform at the tip apex controls single-electron tunneling with combined femtosecond temporal and sub-Å spatial precision. Exploiting this process, single-molecule THz vibrations could be resolved directly in space and time [2]. The mechanism of sub-cycle tunneling control crucially depends on the exact shape of the near-field waveform in the junction, which is determined by interactions of the incoupled terahertz pulses with tip and substrate. To understand the effect of these near-field interactions on the voltage pulses in the junction, we carried out finite element simulations in the frequency domain. The resulting near-field waveforms coincide with experimental results. To further optimize the near-field transients, we study different geometries of the junction.

[1] T. L. Cocker et al., Nature Photon. 7, 620-625 (2013)
[2] T. L. Cocker, D. Peller, P. Yu, J. Repp, and R. Huber,
Nature 539, 263 (2016).

O 50.5 Wed 11:30 H8

Advances with Attosecond Electron Pulse Trains in Ultrafast Transmission Electron Microscopy — •Thomas Rittmann[1], Katharina E. Priebe[1], Christopher Rathje[1,2], Sascha Schäfer[1,2], Sergey V. Yalunin[1], Thorsten Hohage[3], Armin Feist[1], and Claus Ropers[1] — [1]4th Physical Institute - Solids and Nanostructures, University of Göttingen, Germany — [2]Institut für Physik, University of Oldenburg, Germany — [3]Institut für Numerische und Angewandte Mathematik, University of Göttingen

In an ultrafast transmission electron microscope (UTEM), inelastic scattering between a free-electron beam and strong optical near fields [1] allows for a coherent manipulation of the electron quantum state. In this mechanism, the optical field imprints a sinusoidal phase modulation on the electron wave function, which, after subsequent dispersive propagation, results in a temporal electron density modulation [2].

Here, we employ a second electron-light interaction at varied propagation distances with accurately controlled phase delay, and reconstruct the temporal shape of the electron density at each distance with our quantum state tomography algorithm 'SQUIRRELS' [3]. We demonstrate the compression of electron pulses into trains of attosecond bursts and explore the improvement of pulse durations by minimizing phase averaging effects. Such pulse trains will promote new forms of ultrafast electron microscopy with attosecond resolution.

[1] B. Barwick *et al.*, Nature **462**, 902-906 (2009)
[2] A. Feist *et al.*, Nature Physics **12**, 1000-1004 (2016)
[3] K. Priebe *et al.*, Nature Photonics **11**, 793-797 (2017)

O 50.6 Wed 11:45 H8

A versatile setup utilizing shaped optical pulses and time-resolved photoemission electron microscopy to disentangle the ultrafast local response of nanostructured surface systems — •Sebastian Pres[1], Bernhard Huber[1], Daniel Fersch[1], Enno Krauss[2], Daniel Friedrich[2], Victor Lisinetskii[1], Matthias Hensen[1], Bert Hecht[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Nano-Optics & Biophotonics Group, Experimentelle Physik 5, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The possibility to disentangle local field dynamics on nanometer length scales is an important prerequisite for the exploration of interactions between nanostructures and nearby quantum systems.

We combine time-resolved aberration-corrected photoemission electron microscopy, enabling sub-10 nm spatial resolution, with a widely tunable laser source generating sub-20 fs excitation pulses at 1 MHz repetition rate. Phase-stable pulse sequences are formed by liquid-crystal-based pulse shaping and characterised by Fourier-transform spectral interferometry. A detailed knowledge of each pulse sequence's amplitude and phase structure during the measurement allows to quantitatively analyse the influence of the pulse shape and laser spectrum on resulting time-resolved multidimensional spectroscopy signals. Using coherent 2D nanoscopy [1] we investigate local field dynamics within a plasmonic nanoslit resonator.

[1] M. Aeschlimann et al., *Nat. Photonics*, Vol. 9 (2015)

O 50.7 Wed 12:00 H8

Dynamic imaging of plasmonic nanostructures with an ultrafast point-projection electron microscope — •Germann Hergert[1], Andreas Wöste[1], Jan Vogelsang[1], Dong Wang[2], Petra Gross[1], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany — [2]Institut für Werkstofftechnik, TU Ilmenau, 98693, Germany

The motion of electrons inside metallic nanostructures defines their optical properties. The study of this electron motion requires microscopes with few-fs time and nm-spatial resolution. Ultrafast electron microscopy (UEM) is a promising approach towards this goal, combining the spatial resolution of electron microscopes with the temporal resolution of ultrashort laser pulses. So far, the mesoscopic distance between sample and electron emitter limits the temporal resolution in UEM to 100fs.

We solve this problem with a novel electron source in form of a conical gold taper, without direct illumination of the apex. Light is coupled to surface plasmons on the shaft of the tip, which propagate towards the apex, where they cause electron emission.

Implementing this source in our ultrafast point-projection microscope allows minimal sample-emitter distances and therefore enhanced temporal resolution of 20fs [1]. We use this microscope to observe the ultrafast expansion of a photoemitted electron cloud inside a plasmonic nanoresonator in real space, and in addition, we observe a streaking of the probing electrons by the photoemitted charges.

[1] J. Vogelsang et al., Light: Science & Applications 7, 55 (2018)

O 50.8 Wed 12:15 H8

Quantum Pathway Interference between Surface Plasmon Polariton and Photon — •David Janoschka, Pascal Dreher, Michael Horn- von Hoegen, and Frank J. Meyer zu Heringdorf — Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany

It is well known that the coherent superposition of light and surface plasmon polaritons (SPPs) at a surface leads to an interferometric mixture of both their electromagnetic fields. At metal surfaces, electrons can be liberated from this mixture by a nonlinear electron emission pathway. In pump probe experiments, the time dependence of the fields has been used to image the propagation of SPPs in a photoemission electron microscope (PEEM). Strictly speaking, the contrast in the microscope arises from the absorption of either photons, SPPs, or both. Here we use Fourier techniques to disentangle the different contributions of photons and SPPs to the electron emission. In addition to the individual contributions of photons and SPPs we find emission pathways that can only be explained by a quantum interference of SPP and photon.

O 50.9 Wed 12:30 H8

Revealing local mode dynamics within a plasmonic nanoslit cavity by time-resolved photoemission electron microscopy — Bernhard Huber[1], Daniel Friedrich[2], Enno Krauss[2], Sebastian Pres[1], Philipp Grimm[2], Daniel Fersch[1], Julian Lüttig[1], Victor Lisinetskii[1], •Matthias Hensen[1], Bert Hecht[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Plasmonic cavities are known for supporting discrete modes upon resonant excitation with light. The associated characteristic pattern of intense electromagnetic hot-spots can be exploited to enhance light-matter interaction and to enable strong coupling of distinct cavities over a micrometer distance [1] or to strongly couple single excitons and plasmons at room temperature [2]. Here, we disentangle the local field dynamics of individual hot-spots within a nanoslit resonator with a spatial resolution of < 10 nm by combining time-resolved photoemission electron microscopy (PEEM) and a 1 MHz NOPA system. Interestingly, we detect local differences of rather global properties such as the Q-factor and resonance frequency. By using the concept of quasinormal modes we explain these notable local differences, which will be experienced by, e.g., quantum emitters, with a non-negligible influence of adjacent resonator modes.

[1] M. Aeschlimann et al., *Light Sci. Appl.* 6, e17111 (2017)
[2] H. Groß et al., *Sci. Adv.* 4, eaar4906 (2018)

O 50.10 Wed 12:45 H8

Direct optical excitation of dark plasmons for hot electron generation. — •Dominik Höing[1], Niclas Müller[2], Florian Schulz[1], Stephanie Reich[2], and Holger Lange[1] — [1]Institut für Physikalische Chemie, Universität Hamburg, Sedanstraße 19, VG1-045, 20146 Hamburg — [2]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, Raum 1.2.42, 14195 Berlin

Plasmonic gold nanoparticles (AuNP) are of great interest because of their ability to generate hot charge carriers, which can play a key role in photoinduced catalysis [1]. Previous studies have shown that the generation of hot carriers depends on whether or not the photon energy is larger than the threshold for interband transitions while exciting at the plasmon resonance seems to have a low effect [2]. A possible explanation might be a significant contribution of radiative energy losses during the plasmon decay. Dark plasmon modes, which can be observed in AuNP multilayers, do not couple to the far field and might allow to reduce such losses [3]. An experimental access to the efficiency of hot carrier generation is transient absorption spectroscopy. It has proven to be a reliable method as it allows assessing the initial temperature of the electrons after excitation and thermalization [4]. In our contribution we investigate the effect of radiative losses on the excitation of hot electrons, by comparing the hot electron dynamics in AuNP mono- and bilayers.

[1] ACS Cent. Sci. 2017, 3, 482-488 ; [2] J. Phys. Chem. Lett. 2017, 8, 19, 4925-4929 ; [3] ACS Photonics 2018, 5, 10, 3962-3969 ; [4] Chem. Rev. 2011, 111, 3858-3887.

O 50.11 Wed 13:00 H8

Angle-resolved plasmoemission from strong SPP fields — •Pascal Dreher, David Janoschka, Michael Horn-von Hoegen, and Frank Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstrasse 1-21, 47057 Duisburg, Germany

Recent efforts to observe strong-field phenomena in photoemission from metal surfaces have utilized the local enhancement of optical near-fields in nanostructures such as nanotips. On flat metal surfaces high field intensities can be achieved by femtosecond surface plasmon polariton (SPP) pulses. Here we exploit the spatio-temporal nanofocusing of SPPs in Archimedean vortex lenses [1] to achieve particularly strong plasmonic near fields with well-known field distributions on flat Au(111) surfaces. A spectroscopic photoemission electron microscope is employed to detect the electrons which are emitted from the surface by the simultaneous absorption of up to seven SPP quanta. In angle-resolved plasmoemission spectra (ARPLES) we observe signatures which can be attributed to above-threshold plasmoemission from the Au(111) Shockley surface state into SPP-dressed free electron states. The ponderomotive energy that the emitted electrons gain within the strong plasmonic nanofocus is determined from spatially-resolved plasmoemission spectra. The ponderomotive energy provides us with a direct measure for an absolute value of the transverse electric field strength of the SPP in the focus point.

[1] Spektor G, et al., Science 355, 1187 (2017)

O 51: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge V (joint session O/CPP/DS/TT)

Time: Wednesday 10:30–13:15 Location: H9

Topical Talk O 51.1 Wed 10:30 H9

Theoretical Investigations of Electrochemical CO2 Reduction — •Karen Chan — Department of Physics, Technical University of Denmark

The electroreduction of CO_2 has the potential to store energy from intermittent renewable sources and to produce carbon-neutral fuels and chemicals; In this talk, I will discuss new developments in modeling the electrochemical interface. I will then present the application of these models of the interface to CO_2 reduction: the determination of reaction pathways and kinetics on transition metals, field and solvation effects, pH effects on C_2 product selectivity, and implications for catalyst design.

Topical Talk O 51.2 Wed 11:00 H9

First-principles approach to model electrochemical reactions at the solid-liquid interface — •Mira Todorova, Sudarsan Surendralal, and Jörg Neugebauer — MPI für Eisenforschung, Düsseldorf

Processes at solid-liquid interfaces are at the heart of many present day technological challenges related to the improvement of battery materials, electro-catalysis, fuel cells, corrosion and others. Describing and quantifying the underlying fundamental mechanisms is equally challenging for experimental and theoretical techniques.

Utilizing concepts from semiconductor physics, we have developed a novel potentiostat design, which enables us to perform ab initio calculations under controlled bias conditions. Easily applied in standard density functional theory codes, it controls the electrode potential of the system by tuning the excess charge of the working electrode and allows us to obtain direct insight into key mechanisms of electrocatalysis and corrosion. As a prototype example, we consider one of the most corrosive systems under wet conditions - Mg. Using the new approach we solve a 150-year-old problem, which links H-evolution under anodic conditions to Mg dissolution [1].

[1] S. Surendralal, M. Todorova, M.W. Finnis and J. Neugebauer, Phys. Rev. Lett. 120, 246801 (2018).

O 51.3 Wed 11:30 H9

Towards out of the box implicit solvation at liquid-liquid interfaces — •Jakob Filser[1], Markus Sinstein[1], Christoph Scheurer[1], Sebastian Matera[2], Karsten Reuter[1], and Harald Oberhofer[1] — [1]Technische Universität München — [2]Freie Universität Berlin

Implicit solvation models are widely used to incorporate solvent effects in electronic structure theory. Treating the solvent as a structureless dielectric continuum, they lift the necessity to explictly sample solvent degrees of freedom. However, even state of the art models currently cannot treat solvation at technically highly important dielectric interfaces, e.g. between two immiscible liquids.

As a remedy, we modify the multipole expansion (MPE) model to also account for liquid-liquid interfaces, specifically focusing on the electrostatics of mutually interacting dielectric regions. Non-electrostatic free energy contributions thereby are treated with a simple linear model, fitted to experimental free energies of solvation in the two liquids. We demonstrate the efficacy of this approach for small molecules at a water–1-octanol interface, which show the correct qualitative behaviour with respect to orientation and position at the interface.

Future, quantitative applications of our new implicit solvation interface methods are clearly possible but will necessitate both improvements to the non-electrostatic free energy terms and a more exhaustive parameterization effort for a wide range of solvents.

O 51.4 Wed 11:45 H9

Continuum models of the electrochemical diffuse layer in electronic-structure calculations — •Francesco Nattino[1], Oliviero Andreussi[2], and Nicola Marzari[1] — [1]Theory and Simulations of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Department of Physics, University of North Texas, Denton, TX 76207, USA

The electrical diffuse layer is a structure that spontaneously forms at essentially any solvated interface, such that its presence in electrochemistry is ubiquitous. While first-principles methods are desirable to describe any process occurring at the surface, fully-atomistic models of electrolyte solutions suffer from computational limitations. In this context, continuum models represent a practical tool to bypass these difficulties and to account for the presence of the diffuse layer at electrified interfaces. However, despite the increasing popularity of continuum models in the field of materials science, even relatively simple observables such as the differential capacitance (DC) of single-crystal electrode surfaces remain challenging to model quantitatively. I will present and discuss the performance of a hierarchy of continuum diffuse-layer models that we have implemented and coupled to an atomistic first-principles description of a charged metal surface. In particular, I will compare computed DC values for the prototypical Ag(100) surface in an aqueous solution to experimental data, and validate in this way the accuracy of the models considered.

O 51.5 Wed 12:00 H9

***Ab initio* molecular dynamics of Pt(111)/H_2O interfaces in an electrolytic cell setup** — •Sudarsan Surendralal, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany.

Recently, we developed a novel scheme to perform density functional theory (DFT) simulations of electrochemical interfaces under conditions of constant applied voltage utilizing charge transfer from a semiconductor counter electrode [1]. We use a fractionally doped Ne counter electrode because of its inertness, wide band gap, and low deformation potential. Our DFT based molecular dynamics calculations of the Pt(111)/H_2O interface in this setup reveals that we are able to accurately reproduce macroscopic observables like the potential of zero charge (PZC). We discuss the work function drop at the interface at the PZC, due to the charge polarization by the non-dissociative chemisorption of water molecules at the Pt surface. Possible pitfalls due to the choice of the DFT exchange-correlation functional, non-converged computational parameters and confinement effects due to the presence of the counter electrode will also be discussed.

[1] S. Surendralal, M. Todorova, M. W. Finnis, and J. Neugebauer, Phys. Rev. Lett. 120, 246801 (2018).

O 51.6 Wed 12:15 H9

Swipe left for water molecules? - Implicit vs explicit descriptions of liquid water at interfaces. — •Nicolas Hörmann[1], Oliviero Andreussi[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, CH-1015 Lausanne, Switzerland — [2]Department of Physics, University of North Texas, Denton, TX 76207, USA

We present a study of relevant electrochemical interfaces, such as semiconductor-water and metal-water interfaces based on periodic density functional theory (DFT) calculations with the interface modelled with different degrees of complexity. Water at metallic surfaces is modelled within the self-consistent continuum solvation scheme (SCCS) [1] with explicit application of a potential which allows the comparison of pH dependent properties with experimental results [2,3]. In the case of semiconductors, different amounts of interfacial water are substituted with implicit solvent and observables such as the measured band alignment are obtained from thermal averaging over molecular dynamics snapshots. We find that it is necessary and sufficient to include strongly bound interfacial water molecules (dissociated or not) explicitly and replace the rest with an implicit model, in order to obtain consistent results with all-explicit simulations [4]. Based on these result we simulate the surface Pourbaix diagrams of the most stable surfaces of GaAs, GaN, GaP, CdS and anatase and rutile TiO_2.

[1] *J. Chem. Phys.* **136**, 064102 (2012); [2] *Nat Commun.* **9**, 3117 (2018). [2,3] NH (2018) submitted

O 51.7 Wed 12:30 H9

Transition metal oxide nanoparticles as efficient catalysts for proton exchange membrane electrolyzers: morphology, activity and stability — •Daniel Opalka, Yonghyuk Lee, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter — Technische Universität München

Transition metal oxides such as RuO_2 and IrO_2 are currently the best known electrocatalysts for the oxygen evolution reaction from liquid water in proton exchange membrane (PEM) electrolyzers. However, dynamic load operation of PEM cells induces transformations of the catalyst morphology leading to metal dissolution and catalyst degradation. We present a computational model to predict the morphology, activity and stability from *ab initio* electronic structure theory and fundamental thermodynamic principles. Based on this model, we have explored novel strategies to reduce material expenses and improve catalyst stability while preserving high catalytic activity via nanoparticles with a core-shell design. From an analysis of different surface coverages with oxygen, hydroxyl and hydroxo species, voltage-dependent phase diagrams for catalyst surfaces are presented which correlate with characteristic features observed in cyclovoltammetric measurements. Results from atomistic models of selected nanoparticles on the basis of Wulff's Theorem show negligible size effects, but a strong influence of the facet terminations on the surface relaxation.

O 51.8 Wed 12:45 H9

Modelling the fingerprint of chemical reactions on catalytic surfaces in core-electron binding energies — •Johannes Lischner and Juhan Matthias Kahk — Imperial College London

Core-electron X-ray photoemission spectroscopy is a powerful experimental technique to gain information about chemical reactions on catalytic surfaces. Interpreting experimental spectra, however, is often challenging and theoretical modelling of core-electron binding energies is required to meaningfully assign peaks to adsorbate species. In this talk, I will present a novel first-principles modelling strategy to calculate core-electron binding energies of molecules on metallic surfaces. Specifically, we combine plane-wave/pseudoptential DFT calculations of surface slab models for geometry optimizations with all-electron Delta-SCF calculations on cluster models for determining accurate core-electron binding energies. This approach is computationally efficient and yields good agreement with experimental measurements for a wide range of adsorbates on copper(111) surfaces.

O 51.9 Wed 13:00 H9

What Makes a Successful Photoanode? - The Role of the Semiconductor–Catalyst Interface — •Franziska Simone Hegner[1], Benjamin Moss[2], James Durrant[2], Sixto Gimenez[3], José-Ramón Galán-Mascarós[1], and Núria López[1] — [1]Institute of Chemical Research of Catalonia (ICIQ) — [2]Imperial College London — [3]Institute of Advanced Materials, Castellón

A large scale implementations of artificial photosynthesis is still limited by the low efficiencies of the employed photoelectrochemical systems. A common strategy to improve performance is to deposit a co-catalyst on the light-harvesting photoanode. However, the role of the catalyst is controversial; is it acting as a true catalyst, i.e. transferring charges, or is it merely influencing the electronic structure of the semiconductor?[1]

The semiconductor-catalyst interface is key to catalytic performance, but its accurate description is limited since linear scaling relationships no longer apply. Herein the function of the co-catalyst (cobalt hexacyanoferrate) is discussed on two photoanode interfaces, Fe2O3 and BiVO4. Density Functional Theory and time-resolved spectroscopy were used to shed light on the underlying charge-transfer processes. Taking into account the advantages and disadvantages of all applied techniques, a relationship between electronic structure alignment, interface morphology, and photocatalytic efficiency is proposed.[2]

[1] D. R. Gamelin, Nat. Chem., 4 (2012), 965-967. [2] F. S. Hegner, D. Cardena-Moscoros, S. Gimenez, N. López, J. R. Galán-Mascarós. ChemSusChem, 10 (2017) 4552-4560.

O 52: Focus Session: Electron-Phonon Interactions I

Organizers: Lilia Boeri (Sapienza, Rome, Italy) and Claudia Draxl (Humboldt-Universität zu Berlin)

Time: Wednesday 10:30–12:45 Location: H15

Invited Talk O 52.1 Wed 10:30 H15

Electron-boson coupling in correlated materials: a non-equilibrium perspective — •Claudio Giannetti[1], Stefano Dal Conte[2], Giulio Cerullo[2], and Andrea Damascelli[3] — [1]ILAMP, Università Cattolica del Sacro Cuore, via Musei 41, 25121 Brescia, Italy — [2]Department of Physics, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy — [3]Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada

Non-equilibrium techniques are emerging as a unique tool to investigate the coupling of electrons to bosonic degrees of freedom in correlated materials. The recent advances in ultrafast science have paved the way to the study of electron-phonon and electron-spin interactions on their relevant timescales (10-100 fs).

In this talk we will provide an overview of the recent advances in the field and we will discuss the energy relaxation process in conventional anisotropic superconductors and in strongly-correlated materials, with particular focus on superconducting copper oxides.

O 52.2 Wed 11:00 H15

Electron-phonon coupling in laser-induced nonequilibrium states of solids — Tobias Held[1], Sebastian T. Weber[1], Isabel Klett[1], Jan Vorberger[2], and •Baerbel Rethfeld[1] —

[1]Fachbereich Physik und Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern — [2]Institut für Strahlenphysik, Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden

Ultrafast laser pulses heat electrons in solids to highly nonequilibrium distributions. The subsequent energy transfer to the lattice induce nonequilibrium distributions in the phonon system as well. We analyse, how these nonequilibrium states influence the electron-phonon energy transfer as compared to the standard two-temperature model.

Motivated by a nonthermal lattice model [1], we determine the energy transfer from the hot electrons to different phonon modes. The partial Eliashberg functions are obtained with DFT methods, while the relaxation dynamics is traced with help of Boltzmann collision integrals. We also evaluate phonon-phonon scattering terms and examine the phonon relaxation and its influence on the electron-phonon energy transfer [2]. Finally, we show that the electron-phonon scattering can induce a secondary nonequilibrium state in the electron distribution persisting on the timescale of lattice heating [3].

[1] L. Waldecker, R. Bertoni, R. Ernstorfer, J. Vorberger, PRX 6, 021003 (2016).
[2] I. Klett and B. Rethfeld, PRB 98, 144306 (2018).
[3] S.T. Weber and B. Rethfeld, arXiv:1801.06560 (2018).

O 52.3 Wed 11:15 H15

A real space view on the complex renormalization of quasiparticles mediated by electron-phonon interactions — •Jon Lafuente-Bartolome[1,2], Peio Garcia-Goiricelaya[1,2], Idoia G. Gurtubay[1,2], and Asier Eiguren[1,2] — [1]Materia Kondentsatuaren Fisika Saila, University of the Basque Country UPV/EHU, 48080 Bilbao, Basque Country, Spain. — [2]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, 20018 Donostia-San Sebastián, Spain.

We present a novel numerical approach to resolve the real space details of renormalized quasiparticle states and their accompanying virtual phonon cloud in interacting electron-phonon systems. The analytical continuation of the momentum dependent electron self-energy onto the complex-energy plane is performed, where multiple quasiparticle solutions of the Dyson equation can be found. Our method improves previous procedures by overcoming the particle-hole symmetry approximation, and is readily applicable to realistic systems of current interest such as monolayer MoS_2, for which we show some illustrative results.

O 52.4 Wed 11:30 H15

Temperature-dependent optical spectra and band structures using the *ZG*-configuration — •Marios Zacharias and Feliciano Giustino — Department of Materials, University of Oxford, Oxford

Typical calculations of the optoelectronic properties of solids are performed by describing the nuclei as classical particles clamped to their crystallographic positions. This approximation inevitably misses the quantum zero-point motion and thermal effects, as well as phonon-assisted optical processes [1]. Recently we developed a new methodology to incorporate these effects in electronic structure calculations by describing the electron-phonon interaction via the Zacharias-Giustino (*ZG*)-configuration [2]. In this talk I will show the theory behind this *one-shot* method, and I will demonstrate how it can be derived rigorously from the Williams-Lax theory of temperature-dependent electronic transitions [3] in conjunction with the harmonic approximation. I will discuss some recent examples of calculations that have been performed using the *ZG*-configuration, including temperature-dependent band structures and optical spectra of indirect and direct band gap semiconductors. This method holds promise for high-throughput calculations of any property at finite temperature that can be described by the Fermi's Golden rule.
[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).
[2] M. Zacharias, and F. Giustino, *Phys. Rev. B* **89**, 075125 (2016).
[3] M. Zacharias, C. E. Patrick, and F. Giustino, *Phys. Rev. Lett.* **115**, 177401 (2015).

Invited Talk O 52.5 Wed 11:45 H15

Carrier lifetime trends in highly efficient thermoelectrics — •Vidvuds Ozolins — Yale University

Recent developments in electronic structure algorithms based on the Wannier function interpolation of electronic wave functions have enabled accurate first-principles calculations of electron-phonon interactions and intrinsic carrier lifetimes in the relaxation time approximation. This has supplied the final missing piece of the puzzle for predicting the thermoelectric figure of merit $zT = \frac{\sigma S^2 T}{\kappa}$, where the conducrtivity σ, the Seebeck coefficient S, and the total thermal conductivity κ now can all be obtained from the density-functional theory (DFT). This opens up exciting possibilities for theoretically understanding and reliably predicting new materials with high values of zT. We will review several examples from our recent work, including a Li-intercalated analogue of lead telluride (Li_2TlBi), an intermetallic compound with unexpectedly high value of S (CoSi), and a theoretically predicted full Heusler compound with ultrahigh zT (Ba_2BiAu). General factors for high thermoelectric power factors in these compounds include energy dependence of carrier lifetimes for high S, high degeneracy of carrier pockets at the Fermi level, weak electron-phonon scattering for high mobility, and concomitantly low Lorentz numbers for low electronic thermal conductivity.

O 52.6 Wed 12:15 H15

Thermally-Enhanced Fröhlich Coupling in SnSe — •Fabio Caruso, Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin

To gain insight into the peculiar temperature dependence of the thermoelectric material SnSe, we employ many-body perturbation theory and explore the influence of the electron-phonon interaction on its electronic and transport properties. We show that a lattice dynamics characterized by soft highly-polar phonons induces a large thermal enhancement of the Fröhlich interaction. We account for these phenomena in ab-initio calculations of the photoemission spectrum and electrical conductivity at finite temperature, unraveling the mechanisms behind recent experimental data. Our results reveal a complex interplay between lattice thermal expansion and Fröhlich coupling, providing a new rationale for the in-silico prediction of transport coefficients of high-performance thermoelectrics.

O 52.7 Wed 12:30 H15

Fully-Anharmonic, First-Principles Theory of Electronic Transport — •Zhenkun Yuan, Marios Zacharias, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Under typical operation conditions, thermoelectric charge and heat transport are limited by scattering events resulting from electron-phonon coupling (EPC). Although much progress has been made in assessing the respective electronic transport coefficients in the harmonic approximation [1], recent evidence suggests that anharmonic contributions both in the nuclear motion ***and*** the EPCs can play a decisive whereas typically ignored role [2]. We here present a first-principles formalism that fully accounts for these anharmonic effects in electronic transport: Anharmonicity in the nuclear motion is accounted for via *ab initio* molecular dynamics, while anharmonicity in the EPCs is included by evaluating the electronic self-energy along these trajectories in a real-time density-matrix formalism. This gives access to the electronic charge and heat fluxes, enabling us to obtain the thermoelectric transport coefficients via the fluctuation-dissipation theorem. Using both harmonic elemental semiconductors and anharmonic perovskites as example, we discuss the advantages and challenges of the proposed approach.

O 53: 2D Materials II: Transition Metal Dichalcogenides

Time: Wednesday 10:30–13:15 Location: H16

O 53.1 Wed 10:30 H16

Ultrafast Photo-induced Phase Transition in 2D MoTe2 — •Bo Peng — TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — Key Laboratory of Micro and Nano Photonic Structures (MOE), Department of Optical Science and Engineering, Fudan University, Shanghai 200433, China

For phase transition in 2D solids, lots of amazing physical phenomena remain to be understood as compared with the intensively investigated 3D one. A central topic is the nature of photo-induced phase transition in monolayer MoTe2. Using first-principles calculations, we pinpoint that the phase transition from 2H to 1T' phase is induced by purely electronic excitations within several hundred femtoseconds, far shorter than conventional structural phase transition. Such excitation initially changes the chemical bonding. As laser excitation energy is increased to 2 eV, the lattice vibrational modes are softened, leading to symmetry breaking displacements and generating the intermediate structures along the phase transition pathway. The distortions are strongly dependent on laser energy, enabling controllable phase transformation by varying laser wavelength. Our results identify an ultra-rapid and controllable phase transformation mechanism in monolayer MoTe2, opening a new door for precise control of ultra-fast phase transition in low-dimensional systems by tuning laser energy.

O 53.2 Wed 10:45 H16

Angle, spin and time-resolved photoemission spectroscopy on WSe2 — •zakariae el youbi[1,2,4], jakub schüsser[1,3,4], mauro fanciulli[1,4], waly ndiaye[1,4], olivier heckmann[1,4], marie-christine richter[1,4], cephise cacho[2], and karol hricovini[1,4] — [1]LPMS, UCP, Cergy, France — [2]Diamond Light Source, Harwell Campus, Didcot OX11 0DE, UK — [3]Univ. of West Bohemia, Plzeň, Czech Republic — [4]LIDYL-UMR 9222 CEA-CNRS

Tunable bandgap, high specific surface area, fabrication of van der Waals heterojunctions and other specific electronic properties make Transition Metal Dichalcogenides (TMDCs) very promising for the applications in photovoltaics and optoelectronics. In particular WSe2 which is of interest for valleytronic and spintronic device concepts. Here we report the characterization of cleaved WSe2 samples by angle resolved photoemission spectroscopy (ARPES). We measured the band structure of the valence band along Γ - K and Γ - M directions with Helium I and Helium II radiation and as well with ultrashort ($<$ 20 fs) HHG laserlight. Ultrafast dynamics by pump-probe experiments (trARPES) and spin analysis in combination with circular polarised excitation will be discussed.

O 53.3 Wed 11:00 H16

Hyperbolic light dispersion in MoTe2 from many-body perturbation theory: impact of dimensionality — •Saeideh Edalati Boostan, Caterina Cocchi, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Among the transition-metal dichalcogenides, MoTe2 shows only a moderate decrease of photolouminescence intensity with increasing number of layers, which makes it an excellent candidate for opto-electronic applications [1]. Therefore, it is essential to gain insight into the response of this material to electro-magnetic radiation with respect to the number of layers. We investigate the electronic and optical properties of MoTe2, considering a monolayer, a bilayer, and its bulk form. Our study is based on many-body perturbation theory including GW and the Bethe-Salpeter equation (BSE), as implemented in the exciting code [2]. Our BSE results reveal that MoTe2 is a natural type-II hyperbolic material in a window of a few eV between the visible and the ultraviolet (UV) region. We emphasize the importance of including many-body effects for a proper quantitative description of this phenomenon. Going from the monolayer to the bulk, the energy window of hyperbolicity is red-shifted by several tenths of an eV. These findings disclose new perspectives for this material in view of applications in plasmonics and nano-imaging.

[1] I. G. Lezama, et al., Nano Lett. 15 (2015) 2336.

[2] A. Gulans, et al., JPCM 26, 36 (2014).

O 53.4 Wed 11:15 H16

Ultrafast charge transfer in epitaxial WS_2/graphene heterostructures — •Razvan Krause[1], Sven Aeschlimann[1], Antonio Rossi[2,3], Mariana Chavez-Cervantes[1], Stiven Forti[2], Filippo Fabbri[2,4], Camilla Coletti[2,4], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany — [2]Center for Nanotechnology Innovation at NEST, Italian Institute of Technology, Pisa, Italy — [3]NEST, Istituto Nanoscienze, CNR and Scuola Normale Superiore, Pisa, Italy — [4]Graphene Labs, Istituto Italiano di Tecnologia, Genova, Italy

We use time- and angle-resolved photoemission spectroscopy (tr-ARPES) to investigate ultrafast charge transfer in an epitaxial heterostructure made of monolayer WS_2, a direct gap semiconductor with strong spin-orbit coupling, and graphene, a semimetal hosting massless carriers with extremely high mobility. We find that, after photoexcitation at resonance to the exciton in WS_2, the photo-excited holes rapidly transfer into the graphene layer while the photo-excited electrons remain in the WS_2 layer. The resulting charge transfer state is found to have a lifetime of ~1ps [1]. While the overall dynamics can be understood in terms of the relative alignment of the WS_2 and graphene band structures [2], the microscopic mechanism of the observed ultrafast charge transfer remains elusive. We present tr-ARPES data for different pump fluences and pump wavelengths and discuss our results in the context of recent theoretical work on the subject [3,4].

O 53.5 Wed 11:30 H16

Exciton propagation in TMDC monolayers at room temperature — •Marvin Kulig[1], Jonas Zipfel[1], Philipp Nagler[1], Sofia Blanter[1], Jonas Ziegler[1], Christian Schüller[1], Tobias Korn[1], Nicola Paradiso[1], Misha Glazov[2], and Alexey Chernikov[1] — [1]Department of Physics, University of Regensburg — [2]Ioffe Institute, Saint Petersburg, Russian Federation

In our work, we examine two dimensional exciton transport of several TMDC materials by directly monitoring the excitonic emission of the optically excited system through spatially- and time-resolved photoluminescence. In order to suppress effects from the silicon oxide substrate roughness, we additionally produce samples encapsulated between thin layers of hexagonal boron nitride. Depending on the injected exciton density, we observe highly nonlinear behavior with characteristic, qualitative changes in the spatial profiles, which results in an increase of the measured effective diffusion coefficient of up to two orders of magnitude. Solving the diffusion equation in consideration of Auger recombination provides the main interpretation and a physical basis of the observed phenomena. For the encapsulated monolayers, Auger recombination is highly suppressed, while the linear diffusion coefficient is more than one order of magnitude larger than for the as-exfoliated, non-encapsulated monolayers.

O 53.6 Wed 11:45 H16

Spatial extent of the excited exciton states in WS2 monolayers from diamagnetic shifts — •Jonas Zipfel[1], Johannes Holler[1], Anatolie A. Mitioglu[2], Mairana V. Ballotin[2], Philipp Nagler[1], Andreas V. Stier[3], Takashi Taniguchi[4], Kenji Watanabe[4], Scott A. Crooker[3], Peter C. M. Christianen[2], Tobias Korn[1], and Alexey Chernikov[1] — [1]Department of Physics, University of Regensburg D-93053, Germany — [2]High Filed Magnet Laboratory (HFML -EMFL), Radboud University, 6525 ED Nijmegen, The Netherlands — [3]National High Magnetic Field Laboratory, Los Alamos, New Mexcio 87545, USA — [4]National Institute for Materials Science, Tsukuba, Ibaraki 305-004, Japan

Owing to strong Coulomb interactions, the properties of monolayer TMDCs are governed by the formation of tightly bound electron-hole pairs, with binding energies as high as 0.5 eV. This motivates questions of the appropriate description of these exciton states and in particular, their spatial extent. We use magneto-optical reflectance spectroscopy in fields up to 29T to detect energy shifts of exciton ground and excited state resonances in encapsulated WS2 monolayers. These characteristic shifts arise both due to the valley Zeeman and diamagnetic effects. We find similar Zeeman shifts for ground and excited states. An analysis of the diamagnetic shifts allows us to draw direct conclusions on the spatial extent of the exciton states. Exciton radii of about 2nm for the ground and, more importantly, up to 5-8nm for the excited state are obtained, further confirming the applicability of a Wannier-Mott like description of excitons in monolayer semiconductors.

O 53.7 Wed 12:00 H16

Impact of excitons in transition metal dichalcogenides on time-resolved ARPES — •Dominik Christiansen[1], Malte Selig[1], Ermin Malic[2], and Andreas Knorr[1] — [1]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden

Time- and angle resolved photoemission spectroscopy (trARPES) allows to study the dynamics of electronic excitations exploiting the photoelectric effect: A VIS pump pulse creates a non-equilibrium electron occupation dynamics detected by a time delayed XUV probe pulse, examplary performed in ultrathin transition metal dichalcogenides (TMDs) [1]. However, these materials exhibit strongly bound excitons, a complex quasi-particle band structure and their interplay dominate the trARPES spectrum [2].

Here, we develope an excitonic theory of time- and angle resolved photoemission spectroscopy investigating the exciton dynamics at different high symmetry points of the Brillouin zone [3].

[1] R. Bertoni et. al., Phys. Rev. Lett. 117, 277201 (2016)
[2] A. Steinhoff et. al., Nat. Commun. 8, 1166 (2017)
[3] M. Selig et. al., 2D Mater. 5, 035017 (2018)

O 53.8 Wed 12:15 H16

Tensor-Networks for calculating biexcitons in single layered materials — Sandra C. Kuhn and •Marten Richter — Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Germany

The calculation of biexciton states is a numerical very demanding problem due to the high number of involved carriers (two electron-hole pairs). In addition, the rich structure of the Brioullin Zone in two dimensional single layer TMDCs requests an accurate grid on the full Brioullin zone. We show, that a combination of tensor networks with logical circuits lifts this numerical burden and reduce the biexciton problem from a super computer to a workstation problem. Results for excitons and biexcitons in MoS_2 are discussed. Furthermore the method shows potential for future application including quantum dynamics of electron-hole complexes.

[1] S. Kuhn, M. Richter arXiv:1807.09036

O 53.9 Wed 12:30 H16

A many-body view on electronic excitations in TMDCs — •Philipp Marauhn, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Semiconducting transition metal dichalcogenides (TMDCs) have remarkable physical properties. Their two-dimensional nature in the monolayer limit leads to high exciton binding energies of several hundreds of milli-electronvolt. In this talk we discuss effects on the excited states that arise when stacking monolayers into multilayer or bulk systems.

To investigate electronic excitations in TMDCs we employ ab-initio many-body perturbation theory. Notably we solve the Bethe-Salpeter equation on the basis of a preceding LDA+*GdW* calculation, which is a simplified version of the *GW* method. Our results show that screening is a crucial ingredient when describing the optical spectra of TMDCs. Stacking layers on top of each other results in an enhanced screening environment shifting exciton resonances towards lower energy. This redshift is in agreement with experimental differential reflectance measurements [1]. Another effect of stacking is the admixture of pure intralayer excitons with charge transfer configurations.

[1] Y. Niu et al., Nanomaterials, **8**, 725 (2018)

O 53.10 Wed 12:45 H16

De-excitation dynamics in 2D MoS_2 with defects — •Raquel Esteban-Puyuelo[1], Alexey Akimov[2], and Biplab Sanyal[1] — [1]Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Box-516, SE 75120, Sweden — [2]Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, New York 14260-3000, USA

Single layer transition metal dichalcogenides (TMDs), e.g., MoS_2 can be considered as graphene analogues with interesting electronic and optical properties for practical applications, mainly due to their semiconductor nature. Understanding its fundamental properties such as the mechanism of photoinduced de-excitation dynamics is crucial so that TMDs can make the transition from research labs to modern technologies. We have investigated the role of point defects in modifying the direct recombination time of monolayer MoS_2 using time-dependent ab initio non-adiabatic molecular dynamics simulations. We determine which defects would undermine the performance of realistic devices built with this material, as well as the mechanisms behind this effect.

O 53.11 Wed 13:00 H16

Exciton landscape of mono- and bilayer transition metal dichalcogenides — •Thorsten Deilmann and Kristian Sommer Thygesen — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Monolayers and bilayers of transition metal dichalcogenides are intensively studied, in particular due to their rich opto-electronic properties. Until now the main focus has been the investigation of (bright) excitons with zero momentum. In this study we employ *ab initio* many-body perturbation theory within the *GW*/BSE approximation to describe the entire q-resolved exciton band structure for mono- and bilayers of the MX_2 ($M = Mo$, W and $X = Se$, S) TMDCs.

We find that excitonic effects strongly influence the exciton band structure. However, energy differences between extrema with varied exciton momenta can be described fairly well already within DFT.

O 54: Organic Molecules on Inorganic Substrates III: Magnetism, Doping and Interfaces

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

O 54.1 Wed 10:30 H24

Jahn-Teller Splitting in Single Adsorbed Molecules Revealed by Isospin-Flip Excitations — •M. Böhme[1], J. Kügel[1], P.-J. Hsu[1], K. Schneider[1], J. Senkpiel[1], D. Serrate[2], M. Bode[1], and N. Lorente[3] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Germany — [2]Instituto de Nanociencia de Aragon & Departamento Fisica Materia Condensada, University of Zaragoza, Spain — [3]Centro de Fisica de Materiales & Donostia International Physics Center, San Sebastian, Spain

In the past decades, the spin Kondo effect was subject of numerous studies [1]. Its hallmark is a resonance at the Fermi level which emerges from the screening of a spin-degenerate localized orbital and splits in an external magnetic field and leads to inelastic spin-flip excitations. In this study, we report on the observation of an unusual spatial variation of the inelastic STS signal observed on single MnPc molecules adsorbed on $(\sqrt{3} \times \sqrt{3})$ surface alloys of post-transition metals with noble metal fcc(111) surfaces. On these distorted molecules we measure tunneling spectra which are characterized by abrupt rises of the conductance at either positive or negative bias polarity depending on the tip position. The results are interpreted in terms of a Jahn-Teller effect which lifts the orbital degeneracy and leads to an isospin- or pseudospin-flip excitation, the inelastic analogue of an orbital Kondo resonance [2].

[1] M. Ternes *et. al.*, J. Phys. Condens. Matter **21**, 053001 (2009).
[2] J. Kügel *et. al.*, Phys. Rev. Lett. **21**, 226402 (2018).

O 54.2 Wed 10:45 H24

Aromaticity of Contracted Porphyrins: Surface Reactivity of an Adsorbed Corrole — •Jan Herritsch[1], Jan-Niclas Luy[1], Malte Zugermeier[1], Falk Niefind[1], Benedikt P. Klein[1], Martin Schmid[1], Peter Schweyen[2], Martin Bröring[2], Ralf Tonner[1], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Institut für Anorganische und Analytische Chemie, TU Braunschweig, Germany

Corroles belong to the family of cyclic tetrapyrroles. As such, they are related to the well-studied porphyrins, from which they differ by one missing methine bridge and a direct pyrrole-pyrrole link. Thus, they can be described as contracted porphyrins. This small structural difference results in substantial changes, in particular of the delocalized π-electron system. Here, we present a study of the on-surface dehydrogenation reaction of corroles. We have investigated monolayers of an octaalkyl-substituted free-base corrole on Ag(111) and Cu(111) surfaces. The adsorbed molecule contains one labile pyrrolic N-H bond, which dissociates already below 230 K on Ag(111). The barrier of this dehydrogenation was estimated by DFT calculations and is consistent with our experimental results. The valence electronic structure was further characterized by UPS and compared to DFT calculations. The dehydrogenated species, although formally a radical, has almost no remaining spin density in the adsorbed state. By applying the fundamental concepts of aromaticity and electron delocalization, this finding can be explained by charge transfer from the surface to the molecule, so that the aromatic 18π electron system is retained.

O 54.3 Wed 11:00 H24

Study of 12-Metallacrowns-4 Complexes — •Robert Ranecki[1], Swen Ehnert[1], Benedikt Baumann[1], Yaroslav Pavlyukh[1], Georg Lefkidis[1], Wolfgang Hubner[1], Angeliki Athanasopoulou[2], Eva Rentschler[2], Stefan Lach[1], and Christiane Ziegler[1] — [1]Department of Physics, TU Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern — [2]Institute of inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg University Mainz, Duesbergweg 10-14, 55128 Mainz

Organometalic multi spin centers and the orientation of the resulting molecular spin moment break new ground for future applications. In this context, the metallacrown complexes (MC) represent an exceptional class of coordination compounds. In most cases MCs decompose by thermal evaporation which is typically used for ultra-high vacuum preparation. Here, we present the perperation of the 12-MC-4 complex (HNEt3)2[CuCu4(shi)4 on different substrates by e-spray, avoiding a defragmentation of the molecules. Using state-of-the-art quantum-chemistry (beyond the Goodenough-Kanamori rules) enables us to identify the spin split d-states for in situ prepared CuCu4 MC and the electronic molecular structure by photoelectron spectroscopy.For observing metal substrate induced collective spin phenomena we use the hybrid system CuCu4/Cu(100). STM/STS investigations show electronic properties and the adsorption orientation of the CuCu4 molecules related to the lattice of Cu(100).

O 54.4 Wed 11:15 H24

The Mixed Localization of Doping-Induced Charge Transfer at Semiconductor/Organic Interfaces: F4TCNQ on ZnO(10-10) — •Simon Erker and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

At inorganic/organic interfaces, charge transfer occurs in different types, usually depending on the nature of the substrate. On metals, where the adsorbate often hybridizes with the substrate, hybrid bands are formed. These leads to a uniform, fractional charging of the organic overlayer. In contrast, on insulating and inert substrates, charge is transferred as integer electrons, which leads to the coexistence of charged and neutral molecules on the surface. In this work, we use DFT to study the charge distribution in an F4TCNQ monolayer adsorbed on the mixed terminated ZnO surface. Interestingly, we find that both mechanisms appear simultaneously for this system. Upon adsorption, the cyano groups of the molecule bind covalently to surface Zn atoms. The involved molecular orbitals hybridize with the substrate, leading to a homogeneous fractional positive charging of the molecular layer. Introducing free charge carriers in the substrate (e.g. by doping) additionally results in charge transfer of integer electrons into the unhybridized LUMOs of individual molecules. The fraction of molecules with filled LUMOs thereby directly depends on the charge carrier concentration in the ZnO. We conclude that hybridization of the orbitals, and not the "metallicity" of the substrates, determines the charge transfer mechanism.

O 54.5 Wed 11:30 H24

Optoelectronic Properties of Hybrid Systems of Silicon and the Organic Semiconductor Copper-Hexadecafluoro-Phthalocyanine — •Anna Stadlbauer, Hannah Schamoni, and Martin Stutzmann — Walter Schottky Institut, TUM, Garching, Germany

Hybrid systems of organic and inorganic semiconductors combine these two materials in order to benefit from their complementary material properties, e.g.for semiconducting devices like solar cells. Therefore, a detailed knowledge of the electronic properties of the interface between the organic and the inorganic semiconductor is necessary. The organic semiconductor chosen in this work, copper-hexadecafluorophthalocyanine (F$_{16}$CuPc), is air-stable and exhibits n-type semiconducting behavior, and its structural and morphological properties have been investigated by many groups. Besides, several studies have investigated the interaction between metals or other organic semiconductors and F$_{16}$CuPc. Here, thin films of F$_{16}$CuPc are deposited on silicon substrates of different doping types and doping concentrations in an organic molecular beam setup. The resulting hybrid systems are characterized amongst others by current-voltage and Kelvin Probe Force Microscopy measurements. Based on these data, we show the influence of doping concentration and type of the Si substrate on the optoelectronic properties of the hybrid heterojunctions.

O 54.6 Wed 11:45 H24

Influences of potassium-intercalation on molecular properties: DBP on Ag(111) — •Felix Otto[1], Tino Kirchhuebel[1], Anu Baby[2], Bernd Schroeter[1], Roman Forker[1], Guido Fratesi[3], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Department of Materials Science, University of Milano-Bicocca, Via R. Cozzi 55, 20125 Milano, Italy — [3]ETSF and Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria, 16, 20133 Milano, Italy

The polycyclic aromatic hydrocarbon tetraphenyldibenzoperiflanthene (DBP, $C_{64}H_{36}$) has advantageous properties for applications in the field of organic electronics. These are a consequence of its chemical structure consisting of an aromatic backbone with four phenyl rings nearly perpendicular to the molecular plane. We are interested in the effect of potassium intercalation on the structural, optical, and electronic properties of DBP adsorbed on Ag(111). Several structurally reordered stable bonding stages were obtained with K doping. LEED and STM measurements combined with differential reflectance spectroscopy (DRS) as well as XPS and UPS including photoelectron momentum maps (PMMs) were used to investigate the system and yield a variety of different information. These results can only be interpreted unambiguously with the help of DFT calculations. We find that the added K atoms adsorb below the molecule and thereby obstruct the bonding channels between DBP and Ag. A gradual occupation of the DBP LUMO is also observed due to charging by K atoms.

O 54.7 Wed 12:00 H24

Determining Dispersion Relations of strong coupling Metal/Organic Hybrid Structures — •Maximilian Rödel[1], Thomas Stark[2], Jochen Manara[2], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Light matter interaction has been in the focus of intense research in recent years because of its feasibility of tuning the optical properties of sub-wavelength devices and interfaces. In particular, combining nanostructured metallic surfaces with organic semiconducting layers, new coupling phenomena emerge. In this contribution, we investigate the dispersion relations of plexcitons, i.e. of strongly coupled surface plasmons at metallic interfaces and localized excitonic states within a molecular adsorbant layer. For this purpose F$_{16}$ZnPc layers have been chosen due to their strong emission enhancement in close proximity to suited metal surfaces [1]. We demonstrated that the momentum dependent Eigenstates and related energies of the detected plexcitons provide detailed insights in the microscopic characteristics such as coupling strength of $\approx$100 meV or effective interface dielectrics. Furthermore, the role of morphology on the plexciton dispersion is examined by comparing polycrystalline and single crystalline organic layers allowing for an evaluation of their respective potential for innovative opto-electronic devices.

[1] V. Kolb, J. Pflaum, Opt. Express 25 (2017) 6678

O 54.8 Wed 12:15 H24

Addressing the NTCDA/Ag(111) interface state in large unit cells within ab-initio calculations — •Lukas Eschmann, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Molecular adsorption causes interaction between the electronic structure of adsorbate and substrate. One particular case is the energy shift of the Shockley surface state on Ag(111) and other surfaces: upon adsorption of organic molecules the state turns into an interface state leading to a change in dispersion and a shift to higher energy by as much as $\sim 0.5\,\mathrm{eV}$.

Here we address the interface state between the Ag(111) surface and adsorbed NTCDA within density-functional theory (DFT). To identify the dispersion of the interface state we have developed a projection technique which maps the states of the adsorbate system onto the original Shockley state. The projection also handles the loss of the surface periodicity due to the adsorbate, thus recovering the parabolic dispersion of the interface state in its original periodicity. We find that the energy shift of the Shockley state, as well as changes of its effective mass, are proportional to the adsorption coverage. Using our technique we also see a strong anisotropy in the dispersion of the state.

O 54.9 Wed 12:30 H24

Critical Interplay of Atomic and Electronic Structure of Strong Electron Acceptors on Semiconductor Surfaces — •Haiyuan Wang[1], Thorsten Schultz[2], Sergey Levchenko[1], Norbert Koch[2], Matthias Scheffler[1], and Mariana Rossi[1] — [1]Fritz Haber Insitute, Berlin, Germany — [2]Humboldt University, Berlin, Germany

In organic-inorganic interfaces, it is necessary to understand how the atomic and electronic degrees of freedom cooperate or compete to yield the desired functional properties. Here, we address this issue first for strong electron acceptors (F4-TCNQ and F6-TCNNQ) adsorbed on H-Si(111). We perform systematic structure searches using density-functional theory with the HSE06 functional augmented by many-body van-der-Waals corrections. The results show that despite their similar composition, F4-TCNQ and F6-TCNNQ adsorb with significantly different geometries and show island formation propensities consistent with Volmer-Weber and Stranski-Krastanov growth modes, respectively. These densely-packed geometries induce a large interface-charge rearrangement, corresponding to a work-function (WF) increase of 1.11 eV for F4-TCNQ and 1.76 eV for F6-TCNNQ. Interestingly, vibrational fluctuations at room temperature produce a wide distribution of WF values, well modelled by a normal distribution with σ=0.17 eV [1]. Afterwards, we compare these results to the behavior of F6-TCNNQ on MoS_2, where the origin of temperature-dependences in the charge transfer is discussed. This work is supported by the SFB-951 project. [1] H. Wang, *et al.*, arXiv:1811.00037 (2018)

O 54.10 Wed 12:45 H24

Level Alignment in Large-Scale Hybrid Organic-Inorganic Systems from Hybrid Density Functional Theory — •Svenja M. Janke[1], Mariana Rossi[2], Sergey V. Levchenko[3,2], Matthias Scheffler[2], Manoj K. Jana[1], Chi Liu[1], David B. Mitzi[1], and Volker Blum[1] — [1]Duke University, Durham, USA — [2]Fritz Haber Institute of the Max Planck Society, Berlin, GER — [3]Skolkovo Institute of Science and Technology, Moscow, RU

Hybrid organic-inorganic systems allow to combine the properties of organic and inorganic substances at the nanoscale and hence open up a wide area for design of new materials with tunable properties. The positions of carrier levels and their alignment determine electronic properties of hybrid materials. A key challenge is that the systems in question tend to be large, due to alignment of components with inherently different lattice parameters or due to complex crystal structure packing. We here use hybrid density functional theory (FHI-aims all-electron code) for systems comprising over 1,000 atoms to reliably predict level alignments in two types of systems. For the paradigmatic interface system tetracene and pentacene at H/Si(111), we demonstrate the necessity of choosing large cells that reflect the coincidence pattern and find type II heterojunction behavior with potential separation of charge between organic and inorganic component. For a layered double perovskite we demonstrate how level alignment between organic and inorganic compound is affected when the metal ion is exchanged, and rationalize experimentally observed photoluminescence in these systems. Supported by DFG-projects SFB-951, JA 2843/1-1; NSF 1728921.

O 55: Metal Oxide Surfaces III: Adsorption and Reactivity

Time: Wednesday 15:00–17:45 Location: H5

O 55.1 Wed 15:00 H5

Determination of the co-adsorption site of formate and hydroxyls on Fe3O4(001) — •Paul T. P. Ryan[1,2], Tien-Lin Lee[1], David J. Payne[2], and David A. Duncan[1] — [1]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, OX11 0QX UK — [2]Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ

Magnetite nanoparticles are a popular substrate for biofunctionalization, due to their low toxicity and their magnetic moment. These biofunctional materials are typically linked to magnetite via a carboxylate anchoring group. Thus, understanding the adsorption of formic acid on Fe3O4(001) finds continued interest.

A previously published STM and LEED study[1] and unpublished SXRD results[2] show that formic acid dissociatively adsorbs onto the Fe3O4(001) surface at room temperature, resulting in adsorbed formate and hydroxyl species. The prior SXRD measurements clearly indicate bidentate coordination of the formate species, but is insensitive to the surface hydroxyl, whose presence may play a fundamental role in the surface chemistry of Fe3O4(001).

We have exploited the chemical sensitivity of the photoelectron diffraction and X-ray standing wave techniques to directly probe the adsorption of the hydroxyl species, and how it relates to the reconstruction of the magnetite surface. [1] O. Gamba, et al., J. Phys. Chem. C 2015, 119, 35, 20459-20465 [2] B. Arndt, et al., O 55.6 DPG 2018 Berlin

O 55.2 Wed 15:15 H5

Carboxylic acids on magnetite surfaces: insights from DFT — •Kai Sellschopp[1], Björn Arndt[2,3], Marcus Creutzburg[2,3], Heshmat Noei[2], Andreas Stierle[2,3], Stefan Müller[1], and Gregor Vonbun-Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]DESY NanoLab, Deutsches Elektronensynchrotron, Hamburg — [3]Physics Department, Hamburg University

Magnetite (Fe_3O_4) is a versatile material with applications ranging from catalysis over decontamination of water to hybrid materials made from magnetite nanoparticles with organic linker molecules.[1,2] The structure of and interaction with the major surfaces of magnetite plays a crucial role in most of these applications. In this presentation recent work on the adsorption of organic acids at the magnetite (001) and (111) surfaces studied with density functional theory (DFT) is shown. The mechanism behind the structural change of the magnetite (001) surface upon exposure to formic acid is elucidated from a thermodynamics point of view and by comparison to experimental data from surface X-ray diffraction (SXRD). Calculating the vibrational modes, we find that this structural change in turn also affects the vibrational spectrum of the molecule adsorbed at the surface, which also fits to infrared spectroscopy data. Finally, first results on the adsorption of formic acid at the magnetite (111) surface are shown.

[1] G. Parkinson, *Surf. Sci. Rep.* **71**, 272-365 (2016)

[2] A. Dreyer et al., *Nature Materials* **15**, 522-528 (2016)

O 55.3 Wed 15:30 H5

Adsorption of Carboxylic Acids on Magnetite Single Crystal Surfaces — •Marcus Creutzburg[1,2], Heshmat Noei[1], Björn Arndt[1,2], Vedran Vonk[1], Elin Grånäs[1], Kai Sellschopp[3], Gregor Vonbun-Feldbauer[3], and Andreas Stierle[1,2] — [1]DESY NanoLab, Deutsches Elektronen-Synchrotron, Hamburg — [2]Fachbereich Physik, Universität Hamburg — [3]Institute of Advanced Ceramics, Hamburg University of Technology

Magnetite (Fe_3O_4) is an important and diverse transition metal oxide with applications in catalysis, data storage and biomedical imaging. In a recent study, magnetite nanoparticles linked by oleic acid molecules show exceptional isotropic mechanical properties [1]. To give further insight on how these nanoparticles interact with organic molecules, it is crucial to study the flat single crystal surfaces. In this contribution, we present surface X-ray diffraction results in combination with infrared reflection absorption spectroscopy, X-ray photoelectron spectroscopy and scanning tunneling microscopy to investigate the clean magnetite (111) surface and study the adsorption of formic acid and oleic acid on the magnetite (111) and (001) surfaces under UHV conditions.

[1] A. Dreyer *et al.*, Nature Materials **15**, 522-528 (2016)

O 55.4 Wed 15:45 H5

Adsorption of molecules on KTaO3 (001) and their coupling to the 2D electron gas — •Zhichang Wang, Igor Sokolovic, Michael Schmid, Martin Setvin, and Ulrike Diebold — Institute of Applied Physics, TU Wien, Vienna, Austria

The intrinsic polarity of the KTaO3 (001) surface can be compensated in various ways - by defects, surface reconstructions, or a hydroxylated overlayer1. The influence of the polarity on molecule adsorption is a fundamental question with further impact on practical applications. Here, we employ a combined scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) system to study CO adsorption on the bulk-terminated KTaO3 (001) surface. CO preferentially adsorbs on TaO2-terminated terraces and we discuss its possible coupling with 2DEG-like electronic states of the substrate. Two distinctly different adsorption configurations were found, where the corresponding CO molecules show significantly different chemical interaction with the AFM tip, and are arranged in a pattern similar to the electronic standing waves induced by the 2DEG.

Reference: 1. M. Setvin et al., Science 359, 572 * 575 (2018)

O 55.5 Wed 16:00 H5

Acetone on Rutile TiO_2: Studying Adsorption via DFT and FTIRS — Tim Würger[1,2], Kai Sellschopp[1], Wolfgang Heckel[1], Yuemin Wang[3], Heshmat Noei[4], Andreas Stierle[4,5], Stefan Müller[1], and •Gregor Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]MagIC-Magnesium Innovation Centre, Helmholtz-Zentrum Geesthacht — [3]Institute of Functional Interfaces, Karlsruhe Institute of Technology — [4]DESY NanoLab, Deutsches Elektronen-Synchrotron, Hamburg — [5]Physics Department, Universität Hamburg

The adsorption and potential subsequent chemical reactions of acetone on TiO_2 surfaces are highly relevant to various applications ranging from photocatalysis to the formation of hybrid interfaces. In the latter case, acetone may act as a competitor to coupling agents like carboxylic acids. Here, the adsorption geometry, energetics, and vibrational modes of acetone molecules on the rutile TiO_2 (110) surface are studied using density functional theory (DFT). Especially, the importance of sampling the adsorption configuration space and of including non high-symmetry geometries is shown. The computational results are complemented with temperature-dependent ultrahigh-vacuum Fourier transform infrared spectroscopy measurements. At low temperatures the calculated and measured IR spectra agree very well, while upon increasing the temperatures emerging IR bands are seen in the experiments. The modifications of the spectra indicate thermal-induced reactions and their nature is further examined using DFT.[1]

[1] T. Würger et al., *J. Phys. Chem. C* **122**, 19481-19490, 2018

O 55.6 Wed 16:15 H5

Water and methanol adsorption on vicinal ZnO — •Elin Grånäs[1], Björn Arndt[1,2], Michael Busch[3], Fredrik Johansson[4], Christoph Seitz[1], Konstantin Simonov[4], Michael Wagstaffe[1], Anders Sandell[4], Henrik Grönbeck[3], and Andreas Stierle[1,2] — [1]Deutsches-Elektron Synchrotron (DESY), Germany — [2]University of Hamburg, Germany — [3]Chalmers University of Technology, Sweden — [4]Uppsala University, Sweden

Zinc oxide (ZnO) plays an important role in catalysis, where it is often used together with metal nanoparticles in important chemical reactions such as methanol synthesis and low temperature water-gas shift. The detailed reaction mechanisms and role of the ZnO are topics under discussion. Previously we have determined the structure of the bare vicinal ZnO(10-14) surface [1], here we continue with studies of how the under-coordinated Zn- and O-atoms on the surface interact with water and methanol under UHV conditions. Using x-ray photoelectron spectroscopy we have followed the evolution of species present on the surface as a function of coverage and temperature. The distribution of products reveal insights into the influence of the surface steps. Further, based on scanning probe microscopy and surface x-ray diffraction studies we will discuss structural changes occurring upon water exposure.

[1] E. Grånäs, M. Busch, B. Arndt, M. Creutzburg, G. Dalla Lana Semione, A. Schaefer, J. Gustafson, V. Vonk, H. Grönbeck, A. Stierle. "A non-polar, highly reactive vicinal oxide surface". In preparation.

O 55.7 Wed 16:30 H5

Methanol on SrTiO3: adsorption sites and geometry — •Vladyslav Solokha[1,2], Debi Garai[1,3], Axel Wilson[1], Hadeel Hussain[1], Theresia Greunz[2], David A. Duncan[1], Kurt Hingerl[2], and Jörg Zegenhagen[1] — [1]Diamond Light Source Ltd., Didcot, UK — [2]Johannes Kepler University, Linz, Austria — [3]Amity University, Noida, India

Mechanistic understanding of interaction of small organic molecules with oxide surfaces fosters the development of novel oxide-based catalysts. Using I09 beamline[1] at Diamond Light Source, we investigate the surface chemistry of methanol on SrTiO3 (001) from cryogenic to room temperature with a combination of hard and soft X-ray photoelectron spectroscopy (XPS) and x-ray standing waves (XSW). SrTiO3 is a prototypical perovskite and a transition metal oxide posessing (photo)catalytic properties. In our study, we find that methanol dissociates upon adsorption on the surface of strontium titanate forming various species, e.g. methoxy.

In the talk we discuss, adsorption sites and adsorption geometry of methanol and its dissociation products, as evidenced by XPS-XSW.

[1] T.-L. Lee and D. A. Duncan (2018), Synchr. Rad. News, 31:4, 16-22, DOI:10.1080/08940886.2018.1483653

O 55.8 Wed 16:45 H5

STM Reveals the Mechanism of Anatase (001) Nanocatalyst Activation — •William DeBenedetti and Melissa Hines — Cornell University, Ithaca NY, USA

Metal oxide nanocrystals such as TiO_2 have garnered a great deal of attention for environmental remediation applications and photocatalysis. Despite years of study, an atomic-scale picture of the surface chemistry and structure of these materials under operating conditions remains elusive, due to the complex nature of ambient reaction environments. Do these nanocatalysts adopt a bulk-terminated structure in solution environments, or do they reconstruct to minimize their reactivity? Using a newly developed solution-based approach, we will show that shape-controlled crystal growth methods produce films of oriented anatase (001) nanocrystals that are amenable to scanning probe techniques such as STM. Despite being grown in solution and handled in air, the surface of these nanocrystals are surprisingly clean and passivated by a monolayer of fluorine, protecting the surface against adventitious contamination. Using a combination of STM, XPS, and *ab initio* simulations, we will then show that carboxylic acid solutions, the most common TiO_2 functionalization chemistry, cause a spontaneous reorganization of the surface sites, giving rise to a *five-fold increase* in the number of reactive sites on the surface, which reveals a mechanism of nanocatalyst site activation. This structural transformation is not observed in analogous reactions in vacuum and demonstrates the importance of studying these materials under operating conditions.

O 55.9 Wed 17:00 H5

CH-Bond Activation via electronically excited SO_2 on TiO_2-Anatase-(101) and -Rutile-(110).*Ab Initio* Electronic Structure Investigation — •Luca Gerhards and Thorsten Klüner — Carl von Ossietzky Universität, Oldenburg, Germany

The photocatalytic heterogeneous sulfoxidation on titanium dioxides, which requires visible light, seems to be a promising new and more energy efficient alternative to the industrially applied reaction via UV-light.[1,2] Experimental investigations on the mechanism revealed that the adsorption of SO_2 and its electronic excitation lead to a formation of a charge-transfer complex on the surface which catalyzes the subsequent chain reaction.[1] These results stand in contrast to the industrial mechanism and need a deeper investigation. In this contribution, we examine the adsorption and electronic excitation of SO_2 and the CH-bond activation of alkanes on ideal TiO_2-anatase-(101) and -rutile-(110) surfaces from a quantum chemical perspective. Both mechansims (heterogeneous and industrial) will be analysed via high accuracy multireference methods like CASSCF and NEVPT2 to attain a clearer insight into the behavior of this complex radical reaction. An embedded cluster model is designed and compared to calculations with periodic boundary conditions.

[1] F. Parrino, A. Ramakrishnan, H. Kisch, *Angew. Chem. Int. Ed.*, **47**(37), p. 7107-7109, 2008.

[2] R. Graf, *Textilhilfsmittel-Laboratorium der Farbwerke Hoechst*, 50-82, 1952.

O 55.10 Wed 17:15 H5

(Photo-)oxidation Studies on Titania Rutile(110) — •Jessica Kräuter, Lars Mohrhusen, Tim Thiedemann, and Katharina Al-Shamery — Carl-von Ossietzky University of Oldenburg, Institute of Chemistry, Oldenburg, Germany

In chemical industry acetone is produced homogeneously catalysed by the cumene process with explosive peroxides as intermediates.[1] To avoid these, heterogenous catalysed processes are discussed. Earlier work already demonstrated the photo-oxidation of 2-propanol to acetone on MnO, however with low yield.[2] As titania is a well-known photocatalyst, we started model studies under UHV conditions on the interaction of 2 propanol and acetone adsorbed on a rutile TiO$_2$(110) surface. Titania was chosen as recently own work demonstrated the reductive coupling of benzaldehyde and the deoxygenation reaction of methanol which were influenced by bulk defects.[3,4] We have also investigated the effect of oxygen and water coadsorption and tested the photocatalytic performance under UV irradiation. Here, we present Temperature Programmed Reaction Spectroscopy (TPRS) studies to monitor reaction products and polarized Fourier-Transformation Infrared Reflexion Absorption Spectroscopy (FT IRRAS) to identify possible reaction intermediates and their orientation on the surface.

[1] V. M. Zakoshansky, Petroleum Chemistry, 2007, 47, 4, 273. [2] H. Cao, S. L. Suib, J. Am. Chem. Soc., 1994, 116, 5334. [3] P. M. Clawin, C. M. Friend, K. Al-Shamery, A European Journal, 2014, 90, 7665. [4] M. Osmić, L. Mohrhusen, K. Al-Shamery, DOI: 10.1021/acs.jpcc.8b02953.

O 55.11 Wed 17:30 H5

Probing Photoexcited Charge Dynamics of Single Oxygen Vacancies on TiO2(110) at Atomic Scale — •Chaoyu Guo, Xiangzhi Meng, Qin Wang, and Ying Jiang — Peking University, Peking, China

A Titanium dioxide (TiO2) is well known as one of the most widely studied materials in photocatalysis and solar energy conversion. Photoexcited charge dynamics of near-surface defects such as oxygen vacancies plays a critical role in the photocatalytic process of TiO2, but the atomic-scale mechanism is yet to be elucidated. With laser-combined scanning tunneling microscopy, tracking carrier dynamics with high spatial and temporal resolution simultaneously is possible. Here we succeeded to probe the photoexcitation and transient relaxation process of individual oxygen vacancies on rutile TiO2(110) surface. Upon visible-laser illumination, the in-gap states derived from surface oxygen vacancies exhibit prominent downward energy shift accompanied with a suppression of valence tail states, which were attributed to photoexcited electronic transition between the defect levels and conduction band. We found that the photogenerated electrons and holes exhibit rather different carrier dynamics due to the atomic-scale environment variation. Those results shed new lights onto the visible photoresponse of reduced-TiO2 materials and reveal the influence of atomic defects on the electron-hole recombination dynamics in real space.

O 56: Plasmonics & Nanooptics IV: Materials Science and Chemistry Applications (joint session O/CPP)

Time: Wednesday 15:00–17:45 Location: H8

O 56.1 Wed 15:00 H8

Switching between sharp Mie and broad plasmonic resonances in phase-change material metasurfaces — •Sophia Wahl, Andreas Hessler, Matthias Wuttig, and Thomas Taubner — Institute of Physics (IA) RWTH Aachen

Active metasurfaces (MSs) based on phase-change materials (PCMs) enable versatile compact optics like tunable metalenses [1]. PCMs can be rapidly and reversible switched between their amorphous and crystalline phases which is accompanied by a pronounced non-volatile change in their optical properties [2]. Commonly, PCMs integrated in MSs feature a large change in their positive permittivity.

We present how the phase-change material In$_3$SbTe$_2$ (IST) can be used to switch resonators in an infrared (IR) MS between sharp Mie resonances and broad plasmonic resonances. In the IR, the permittivity of IST changes from positive to negative upon crystallization, effectively switching from dielectric to metallic. We demonstrate how this can be used to dramatically change the resonance width and the resonance frequency of IR resonators.

Our work opens up new design concepts for applications like active spectral filters and absorbers, because it could provide tunable bandwidth and operation frequency at the same time.

[1] X. Yin et al., Light: Science & Applications 6, e17016 (2017)
[2] M. Wuttig et al., Nano Photon. 11, 465 (2017)

O 56.2 Wed 15:15 H8

Infrared nanoscopy to unravel the influence of defects in resistive switching of In$_3$SbTe$_2$ — •Niklas Eicker[1], Martin Lewin[1], Raimondo Cecchini[2], Sebastian Walfort[1], Matthias Wuttig[1], Martin Salinga[1], Massimo Longo[2], and Thomas Taubner[1] — [1]RWTH Aachen - Institute of Physics (1A) — [2]CNR - IMM

Phase change materials (PCMs) exhibit at least two stable states at room temperature, one crystalline and one amorphous. Characteristically the different states show a high electrical and optical contrast which can be used for fast, energy efficient and non-volatile nano switches [1]. Thus PCMs are a promising material class for persistent memory devices like PCRAM.

Scattering-type scanning near-field optical microscopy (s-SNOM) in the infrared spectral range can be used to study the differences in local conductivity of both states [2]. Opposed to other techniques like TEM, SNOM allows to study the same system in different states without sample preparation or damaging the PCM.

To investigate the influence of defects on phase change processes in highly scaled PCM devices, we electrically contacted and switched PCM nanowires [3]. With infrared s-SNOM we revealed strong inhomogeneities, which might be linked to a reduced local conduction due to structural defects.

[1] M. Wuttig et al., Nat. Mater. 6, 824 (2007)
[2] M. Lewin et al., Appl. Phys. Lett. 107, 151902 (2015)
[3] S.Selmo et al., Appl. Phys. Lett. 109, 213103 (2016)

O 56.3 Wed 15:30 H8

Switchable absorber/emitter based on vanadium dioxide — •Xinrui Lyu[1,2,3], Taubner Thomas[1], and Yunzhen Cao[2] — [1]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]Key Laboratory of Inorganic Coating Materials CAS, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, PR China — [3]University of Chinese Academy of Sciences, Beijing 100049, PR China

We numerically demonstrate a switchable metamaterial absorber/emitter based on vanadium dioxide (VO2). The absorber consists of three layers, top patterned VO2 layer, dielectric spacer layer and bottom reflective layer. Perfect absorption can be thermally turned on when the excitation of magnetic resonance is supported with the metallic VO2, while switched off with semiconducting VO2. The absorption peak can be tuned with different shapes and geometries of patterned VO2 layer. The absorption bandwidth can be largely broadened when using lossy metallic VO2 instead of noble metal as reflective layer. The results would facilitate the design of switchable metamaterials for active control in energy and sensing applications.

O 56.4 Wed 15:45 H8

Tip-enhanced Raman spectroscopy of ultrathin ZnO layers on Ag(111) — •Shuyi Liu[1], Martin Wolf[1], and Takashi Kumagai[1,2] — [1]Department of Physical Chemistry, Fritz-Haber Institute of the Max-Planck Society, Faradayweg 4-6, 14195 Berlin, Germany. — [2]JST-PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan.

Tip-enhanced Raman spectroscopy (TERS) is a powerful nanoscale vibrational microspectroscopy combining high-spatial resolution of SPM with chemical sensitivity of surface enhanced Raman spectroscopy [1, 2, 3]. We report the TERS measurement of the ultrathin ZnO layers epitaxially grown on a Ag(111) surface. The enhancement mechanisms were examined in detail by a combination of STS and STM-induced luminescence spectroscopy with the TERS measurements. We found a clear correlation between the TERS signal and the plasmonic properties of the STM junction. It was also revealed that the TERS intensity increases exponentially with decreasing the tip-surface distance and the decay constant is largely different inside and outside the tunneling regime. Our results provide a detailed insights into the TERS mechanism and the plasmonic properties relevant for field enhancement and confinement in nanoscale cavities. References [1] Annu. Rev. Phys.

Chem. 63, 379 (2012). [2] Chem. Rev., 117, 4961-4982 (2017) [3] Chem. Soc. Rev., 46, 4020 (2017).

O 56.5 Wed 16:00 H8

Dependence of graphene photoluminescence blinking on the local field enhancement — Markus Pfeiffer[1], •Mo Lu[1], Boris V. Senkovskiy[2], Danny Haberer[3], Felix R. Fischer[3], Fan Yang[2], Klaus Meerholz[1], Yoichi Ando[2], Alexander Grüneis[2], and Klas Lindfors[1] — [1]Department of Chemistry, University of Cologne, Luxemburger Str. 116, D-50939, Köln, Germany — [2]II. Physikalisches Institut, University of Cologne, Zülpicher Strasse 77, 50937 Köln, Germany — [3]Department of Chemistry, University of California at Berkeley, Tan Hall 680, Berkeley, CA 94720, USA

Armchair-edge graphene nanoribbons (AGNRs) are novel one-dimensional semiconductors with well-defined structure and promising optoelectronic properties. Their nanometer-sized dimensions and versatile electronic properties make them the ideal candidate for future optoelectronics. By coupling GNRs to plasmonic nanoantennas array, we obtain an enhancement of photoluminescence and Raman scattering intensity [1]. In the hotspots of the antennas, we observe the blinking of emission from AGNRs, which is a typical characteristic of a single quantum emitter [2]. Here we study the influence of the local field enhancement on the blinking process and find that the amplitude of the blinking events strongly correlates with the enhancement.

Reference:

[1] M. Pfeiffer, et al. 2D Materials, 5, 045006 (2018)

[2] M. Pfeiffer, et al. Nano Lett. 18, 7038-7044 (2018)

O 56.6 Wed 16:15 H8

Electrochemistry on Copper Nanostructures for Active Plasmonics — •Annette Böhme, Florian Sterl, Elinor Kath, Monika Ubl, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Applications of active plasmonics include the development of advanced plasmonic color displays and switchable metasurfaces. We aim to fabricate plasmonic nanostructures that can be switched electrochemically by applying a voltage.

Copper is a suitable material for this attempt as it can easily be switched electrochemically between copper (Cu) and copper oxide (CuO/ Cu_2O) [1]. We have developed a manufacturing process to fabricate high-quality inverse copper nanostructures that exhibit well-modulated plasmonic resonances. We use these samples to perform cyclic voltammetry in order to switch them electrochemically, and at the same time we perform spectral reflectance measurements in the visible wavelength range. Thereby, we demonstrate that the resonances can be reversibly shifted by as much as 80 nm. The wavelength shift becomes stronger after several cycles of voltammetry which we attribute to the modification of the copper surface with repeated oxidation and reduction.

These results provide a basis for the future development of pixelated active plasmonic devices.

[1] Ye Wan, Yundian Zhang, Xianle Wang, and Qing Wang, Electrochem. Commun. 36, 99 (2013).

O 56.7 Wed 16:30 H8

How Metal Nanoantennas' Optical Properties Affect Surface Enhanced Infrared Absorption — •Michael Tzschoppe, Christian Huck, Jochen Vogt, Frank Neubrech, and Annemarie Pucci — Kirchhoff Institute for Physics, Heidelberg University, Germany

Surface enhanced infrared absorption (SEIRA) is known as a powerful tool to study tiny amounts of molecules on the basis of enhanced vibrational signals. In order to further increase the enhancement, the impact of the structures' geometry as well as their interaction have been intensively investigated within the last decade.[1,2] We present an experimental study with focus on the impact of the nanoantennas' metal-optical properties on SEIRA sensitivity. Various aspect ratios of nanoantennas made of the metals gold, silver, copper, aluminum, and iron, respectively, were inspected. From the measured fundamental plasmonic resonance spectra the contributions of the intrinsic damping (electron scattering) as well as the radiative damping (light scattering) were evaluated. The SEIRA enhancement factors were determined for a thin organic probe layer. These investigations finally yield the correlation between the ratio of intrinsic damping and radiation damping with the SEIRA enhancement, which clearly shows the maximum enhancement when both damping mechanisms contribute equally.[3]

[1] Neubrech *et al.* Chem. Rev. **2017**, 117 (7), 5110

[2] Dong *et al.* Nano Lett. **2017**, 17 (9), 5768

[3] Tzschoppe *et al.* J. Phys. Chem. C **2018**, 122 (27), 15678

O 56.8 Wed 16:45 H8

Watching a single fluorophore molecule walk into a plasmonic hotspot — Ling Xin[1,2], •Mo Lu[3], Steffen Both[4], Markus Pfeiffer[3], Maximilian J. Urban[1,2], Chao Zhou[1,2], Hao Yan[5], Thomas Weiss[4], Na Liu[1,2], and Klas Lindfors[3] — [1]Max Planck Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany — [2]Kirchhoff Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany — [3]Department of Chemistry, University of Cologne, Luxemburger Straße 116, 50939 Köln, Germany — [4]4th Physics Institute and Stuttgart Research Center of Photonic Engineering, University of Stuttgart, 70569 Stuttgart, Germany — [5]Department of Chemistry & Biochemistry, Biodesign Institute, Arizona State University, Tempe, AZ 85287-5601, USA

Plasmonic nanoantennas allow for enhancing the spontaneous emission, altering the emission polarization, and shaping the radiation pattern of quantum emitters. A critical challenge for the experimental realizations is positioning a single emitter into the hotspot of a plasmonic antenna with nanoscale accuracy. We demonstrate a dynamic light-matter interaction nanosystem enabled by the DNA origami technique. A single fluorophore molecule can autonomously and unidirectionally walk into the hotspot of a plasmonic nanoantenna along a designated origami track. Successive fluorescence intensity increase and lifetime reduction are in situ monitored using single-molecule fluorescence spectroscopy. Our scheme offers a dynamic platform, which can be used to develop functional materials, investigate intriguing light-matter interaction phenomena as well as to serve as examine theoretical models.

O 56.9 Wed 17:00 H8

Surface-enhanced infrared absorption spectroscopy for in-vitro detection of the polypeptide monolayer conformation on a single gold nanoantenna — •Rostyslav Semenyshyn[1,2], Florian Mörz[1,2], Frank Neubrech[1,3], and Harald Giessen[1,2] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart — [2]Center for Integrated Quantum Science and Technology, IQST — [3]Kirchhoff Institute for Physics, University of Heidelberg

In our present work, we demonstrate the capability of surface-enhanced infrared absorption spectroscopy for ultra-sensitive in-vitro detection of the secondary structure of polypeptides monolayer. We utilized a monolayer of thiols as a bonding spacer for deposition of poly-L-lysine (PLL) molecules onto the gold surface [1]. We tuned the length of nanoantennas to be resonant at the frequency of the amide-I band of PLL and performed SEIRA measurements in the D_2O environment using a specially designed transmittance flowcell. To measure an optical response of a *single* nanostructure, we pushed our system towards the diffraction limit and therefore applied a light source with higher brilliance, namely specifically designed broadband tunable laser [2]. Then, we compare our results to a globar, as well as a synchrotron, which are well-known FTIR light sources. With further advances it might become possible to scale the process down to a few or even single proteins.

[1] R. Semenyshyn, M. Hentschel, C. Stanglmair, T. Teutsch, C. Tarin, C. Pacholski, H. Giessen, and F. Neubrech, Nano Lett. (2018); doi: 10.1021/acs.nanolett.8b02372 [2] T. Steinle, F. Mörz, A. Steinmann, and H. Giessen, Opt. Lett. 41, 4863 (2016)

O 56.10 Wed 17:15 H8

Optical Nanoplasmonic CO2 Detection in the Visible by Polyethylenimine — •Pohl Tobias, Sterl Florian, Strohfeldt Nikolai, and Giessen Harald — 4th Physics Institute and Research Center SCOPE, University of Stuttgart, 70569 Stuttgart, Germany

In industrial production and other technologically relevant processes CO2 is a common byproduct that must be monitored to keep up a high efficiency. Most of the currently available CO2 detection systems use an electrical readout. This poses in environments with explosive or flammable gases a major risk of spark ignition. The available optical solutions, which circumvent this risk altogether, rely on the characteristic infrared absorption of CO2. While being very specific this method requires a large sensing volume. In our contribution, we introduce a cheap and compact nano-optical gas detection scheme for CO2 based on a plasmonic perfect absorber structure combined with the polymer polyethylenimine. The polymer acts as the gas sensitive part as it changes its refractive index by absorbing CO2, which is then translated by the absorber to a resonance shift. By tracking the plasmon resonance we studied the time, concentration, and temperature dependence, as well as possibilities to enhance the response and aging effects. Furthermore we will show that this sensing scheme also works with a much simpler setup consisting only of a LED, a photodiode, and appropriate electronics.

O 56.11 Wed 17:30 H8

three-dimensional plasmonic nanostructure design for boosting photoelectrochemical — •rui xu, huaping zhao, max sommerfeld, and yong lei — Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693, Ilmenau, Germany

Plasmonic nanostructures have been widely incorporated into different semiconductor materials to improve solar energy conversion. An important point is how to manipulate the incident light so that more light can be efficiently scattered and absorbed by the semiconductors. Here, by using a tunable three-dimensional Au pillar/truncated-pyramid (PTP) array as a plasmonic coupler, a superior optical absorption of about 95% within a wide wavelength range is demonstrated from an assembled CdS/Au PTP photoanode. Based on incident photon to current efficiency measurements and the corresponding simulations, it is concluded that the enhancement is mainly attributed to an appropriate spectral complementation between surface plasmon resonance modes and photonic modes in the Au PTP structure over the operational spectrum. Because both of them are wavelength dependent, the Au PTP profile and CdS thickness are further adjusted to take full advantages of the complementary effect and subsequently, an angle independent photocurrent with an enhancement of about 400% was obtained. The designed plasmonic PTP nanostructure of Au is highly robust and it could be easily extended to other plasmonic metals equipped with semiconductor thin film for photovoltaic and photoelectrochemical cells.

O 57: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge VI (joint session O/DS/CPP/TT)

Time: Wednesday 15:00–17:45 Location: H9

O 57.1 Wed 15:00 H9

First-principles quantum transport simulations including strong correlation effects — •Andrea Droghetti[1], Wilhelm Appelt[2], Liviu Chioncel[2], Milos Radonjić[3], Enrique Muñoz[4], Stefan Kirchner[5], David Jacob[1], Dieter Vollhardt[2], Angel Rubio[6], and Ivan Rungger[7] — [1]University of the Basque Country (Spain) — [2]University of Augsburg (Germany) — [3]University of Belgrade (Serbia) — [4]Pontificia Universidad Católica de Chile — [5]Zhejiang University (China) — [6]Max Planck Institute for the Structure and Dynamics of Matter (Germany) — [7]National Physical Laboratory (UK)

When magnetic molecules are brought into contact with metals the electron-electron interaction leads to the appearance of the correlated Kondo state. In this talk we will present the results of first-principles calculations for the electronic structure and the linear-response conductance of radical molecules adsorbed on metallic surfaces in the Kondo regime [Phys. Rev. B 95, 085131 (2017), Nanoscale 10, 17738 (2018)]. In particular we will outline the methodological approach as implemented in the Smeagol electron transport code and we will benchmark the results against experiments. The method relies in the first place on the combination of Density Functional Theory with the Green's functions technique. We will explain how a molecular devices is projected onto an effective Anderson impurity problem, which is then solved either by continuum time quantum Monte Carlo or numerical renormalization group. Finally, we will describe some work-in-progress aimed at computing transport properties beyond linear-response.

O 57.2 Wed 15:15 H9

Density functional theory for transport through correlated systems — •Stefan Kurth — Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — Donostia International Physics Center DIPC, San Sebastian, Spain

A recently proposed density functional formalism to describe electronic transport through correlated systems in the steady state uses both the density on the junction and the steady current as basic variables. The corresponding Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias, which are universal functionals of the basic variables.

A recent parametrization of the xc potentials for the single-impurity Anderson model correctly incorporates both the Kondo and Coulomb blockade regimes. It allows for calculation of currents and differential conductances at arbitrary bias and temperature at negligible numerical cost but with the accuracy of sophisticated renormalization group methods. A time-local version of this functional is used to study the Anderson model under the influence of both DC and AC biases. We observe interaction-induced shifts of the photon-assisted conductance peaks, supression of the Kondo plateau at zero temperature and lifting of Coulomb blockade at finite temperature.

O 57.3 Wed 15:30 H9

Exact factorization of the many-electron wave function — •Camilla Pellegrini[1], Antonio Sanna[1], and Eberhard K. U. Gross[1,2] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — [2]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

The exact factorization approach [1], originally developed for a system of electrons and nuclei, is extended to a system of electrons only. This allows for a two-particle Schroedinger equation, which uniquely defines the exact effective interaction between two electrons in the medium. This interaction differs from the effective interaction, W, used in many-body Green's function techniques. In particular, it is spin-dependent. We illustrate the formalism for the simplest case of exchange interactions only.

[1] A. Abedi, N.T. Maitra, E.K.U. Gross, PRL 105, 123002 (2010).

O 57.4 Wed 15:45 H9

Many-body spectral functions from steady state density functional theory — •David Jacob[1,2] and Stefan Kurth[1,2,3] — [1]Dpto. de Física de Materiales, Universidad del País Vasco UPV/EHU, San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]DIPC, San Sebastián, Spain

We present a scheme to extract the true many-body spectral function of an interacting many-electron system from an equilibrium density functional theory (DFT) calculation [1]. To this end we devise an ideal STM-like setup and employ the recently proposed steady-state DFT formalism (i-DFT) which allows to calculate the steady current through a nanoscopic region coupled to two biased electrodes [2]. In our setup one of the electrodes serves as a probe ("STM tip"). In the ideal STM limit of vanishing coupling to the tip, the system to be probed is in quasi-equilibrium with the "substrate" and the normalized differential conductance yields the exact equilibrium many-body spectral function. Moreover, from the i-DFT equations we derive an exact relationship which expresses the interacting spectral function in terms of the Kohn-Sham one. Making use of i-DFT xc functionals that capture Coulomb blockade as well as Kondo physics, the method yields spectral functions for Anderson impurity models in good agreement with NRG calculations. It is thus possible to calculate spectral functions of interacting many-electron systems at the cost of an equilibrium DFT calculation.

References: [1] D. Jacob and S. Kurth, Nano Lett. **18**, 2086 (2018) [2] G. Stefanucci and S. Kurth, Nano Lett. **15**, 8020 (2015)

O 57.5 Wed 16:00 H9

Magnetic phase transitions induced by pressure and magnetic field: the case of antiferromagnetic USb2 — •Leonid Sandratskii — Max Planck Institute of Microstructure Physics, Halle, Germany

Fascinating phenomena observed under applied pressure and magnetic field are currently attracting much research attention. Recent experiments have shown that application of the pressure or magnetic field to the USb2 compound induce the transformations of the ground-state antiferromagnetic (AFM) up-down-down-up structure to, respectively, ferromagnetic (FM) or ferrimagnetic configurations. Remarkably, the magnetic critical temperature of the FM state, induced by pressure, is more than two times smaller than the Neel temperature of the ground state. We performed density-functional theory (DFT) and DFT+U studies to reveal the origin of the unusual magnetic ground-state of the system and the driving mechanisms of the phase transitions. We investigate both the magnetic anisotropy properties and the parameters of the interatomic exchange interactions. To study pressure-induced effects we carry out calculations for reduced volume and demonstrate that the AFM-FM phase transformation indeed takes place but depends crucially on the peculiar features of the magnetic anisotropy. We also explain why the magnetic field that couples directly to the magnetic moments of atoms leads to the phase transition to the ferrimagnetic state whereas the pressure that does not couple directly to magnetic moments results in the FM structure.

O 57.6 Wed 16:15 H9

Charge localization at a weakly coupled molecule-metal system studied by linear expansion Δ-self-consistent field density-functional theory (ΔSCF-DFT) — •Hadi H. Arefi[1,2], Daniel Corken[3], Reinhard Maurer[3], F. Stefan Tautz[1,2], and Christian Wagner[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Department of Chemistry, University of Warwick, Coventry, United Kingdom

Predicting the charge arrangements at the interface between molecules and metals represents a formidable challenge for semi-local approximations to Density Functional Theory (DFT). This could become even more critical when molecules are only weakly coupled to the metal. Single-molecular devices based on such weak coupling have recently been created by molecular manipulation with a scanning probe microscope (SPM), where a single PTCDA (perylene-tetracarboxylic dianhydride) molecule was placed in a free-standing upright configuration either on a SPM tip [1] or on a pedestal of two adatoms on the Ag(111) surface [2]. There are indications that the mechanism stabilizing these unexpected configurations is linked to an integer charge transfer creating a singly occupied molecular orbital. We use the ΔSCF-DFT method [3] to confine charge on the LUMO of the PTCDA and study the consequences with vdW-corrected DFT.

[1] C. Wagner et al. Phys. Rev. Lett. 115, 026101 (2015) [2] T. Esat et al. Nature 558, 573 (2018) [3] R. J Maurer, K. Reuter, JCP 139, 014708 (2013)

O 57.7 Wed 16:30 H9

Dispersion corrected density functional theory studies on PVDF/hydrated aluminium nitrate composite system — •Ranjini Sarkar and Tarun Kundu — Indian Institute of Technology, Kharagpur

Electro-active polymer Polyvinylidene fluoride (PVDF) based ferroelectric composites have gained significant technological importance over conventional ceramic ferroelectrics. This article provides quantum chemical description of PVDF/ hydrated aluminium nitrate salt composite system in the light of density functional theory. Four monomer units of pristine α and β-PVDF, pure Al(NO3)3.9H2O, and PVDF/ Al(NO3)3.9H2O structures are optimized using dispersion corrected exchange correlation functional B3LYP-D and 6-311+G(d,p) basis set. Similar to the experimental findings, the current theoretical investigation also suggests that hydrogen bond interaction between PVDF and the hydrated salt molecule plays the major role for the enhancement of ferroelectric properties in this composite system. Non-covalent interaction phenomenon is elucidated on the basis of natural bond orbital analysis, Bader's quantum theory of atoms in molecules and reduced density gradient analysis. Chemical Reactivity and charge transfer mechanisms are explained using atomic-dipole corrected Hirshfeld population analysis, molecular electrostatic potential plot and frontier molecular orbital analyses, respectively.

O 57.8 Wed 16:45 H9

Band-structure effects in vertical layered material heterostructures — •Nicholas D. M. Hine[1], Gabriel C. Constantinescu[2], Nelson Yeung[1], Siow-Mean Loh[1], José María Escartín[2], Cuauhtemoc Salazar Gonzalez[1], and Neil R. Wilson[1] — [1]Department of Physics, University of Warwick, United Kingdom — [2]Cavendish Laboratory, University of Cambridge, 19 JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Controlling the properties of layered material heterostructures is crucial to the success of devices based on the novel capabilities of 2D materials, yet theoretical insight has been limited by the large system sizes required to study rotated, incommensurate interfaces. We use linear-scaling DFT calculations with non-local vdW functionals to explore large-scale models of heterostructures of interest for device applications. Results will be presented for heterostructures including MoS2/MoSe2, MoSe2/WSe2, and other Transition Metal Dichalcogenide pairings, TMDCs with graphene and hBN substrates, and hBN/Phosphorene. Band-structure changes caused by stacking and rotation of the layers are obtained by unfolding the supercell spectral function into the primitive cells, incorporating spin-orbit coupling. Changes in spectral weight and band-structure between the monolayers and heterostructured interfaces show how lattice mismatch (MoS2/MoSe2) or spacer layers (Phosphorene/hBN/Phosphorene) can allow the component monolayers to retain more independence in heterostructures than in homo-stacks. Finally, applying electric fields allows the behaviour of gated structures to be predicted and explained.

O 57.9 Wed 17:00 H9

Global Trends in Calcium-Silicate-Hydrate Phases Identified by Infrared Spectroscopy and Density Functional Theory — •Mohammadreza Izadifar, Franz Königer, Andreas Gerdes, Christof Wöll, and Peter Thissen — Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Building and construction industry are at the same time the backbone and the driving force of our modern society. Nearly all our today's technical infrastructure is based on cement-based materials. Detailed, spectroscopic investigations of model reactions on well-defined mineral substrates under UHV-conditions are largely lacking, thus prohibiting a validation of theoretical methods. Eight different Calcium-Silicate-Hydrate (CSH) phases, namely Tobermorite 14Å, Tobermorite 11Å, and Tobermorite 9Å, Wollastonite, Jaffeite, Jennite, γ-C2S, and α-C2SH, are calculated with the help of Density Functional Theory using the Vienna ab initio simulation package (VASP). First, we take care of the mechanical properties of the material. Our results revealed that Jaffeite, γ-C2S, and α-C2SH have a linear bulk modulus due to the monomer structure of silicate tetrahedra. Tobermorite 14Å and Jaffeite have the lowest and highest bulk modulus, respectively. In the second part, the optimized geometries allow for the precise calculations vibrational eigenmodes and frequencies by the force-constant (FC) approach. The proportions of C/S and H/C are major criteria for the classification of the calculated wavenumber of ν(Si-O) for all phases in our model system.

O 57.10 Wed 17:15 H9

Origin of carbon 1s binding energy shifts in amorphous carbon materials — •Michael Walter[1,4,5], Filippo Mangolini[2], Robert W. Carpick[3], and Michael Moseler[4,5] — [1]FIT, University of Freiburg, Germany — [2]University of Texas at Austin, USA — [3]University of Pennsylvania, USA — [4]Fraunhofer IWM, Freiburg, Germany — [5]Physikalisches Institut, Universität Freiburg, Germany

The quantitative evaluation of the carbon hybridization state by X-ray photoelectron spectroscopy (XPS) has been a surface-analysis problem for the last three decades due to the challenges associated with the unambiguous identification of the characteristic binding energy values of sp^2- and sp^3-bonded carbon. Here, we compute the binding energy values for model structures of various carbon allotropes, including graphite, diamond, doped-diamond, and amorphous carbon (a-C), using density functional theory (DFT). The large band-gap of diamond allows defects to pin the Fermi level, which results in large variations of the C(1s) core electron energies for sp^3-bonded carbon, in agreement with the large spread of experimental C(1s) binding energy values for sp^3 carbon. In case of hydrogen-free a-C, the C(1s) core electron binding energy for sp^3 carbon atoms is approximately 1 eV higher than the binding energy for sp^2-hybridized carbon. However, the introduction of hydrogen hinders the unambiguous quantification of the carbon hybridization state on the basis of C(1s) XPS alone. This work can assist surface scientists in the use of XPS for the accurate characterization of carbon-based materials.

O 57.11 Wed 17:30 H9

Mechanically tuned conductivity of graphene grain boundaries from first-principles calculations — Delwin Perera, •Jochen Rohrer, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Nanocrystalline graphene has recently been shown to have a strong piezoresistivity and strain gauge factors that are notably higher compared to single- or microcrystalline graphene [1]. The origin of the enhanced piezoresistivity in nanocrystalline graphene is still not fully understood, but several theoretical works suggest that grain boundaries are the main cause as these can evoke transport gaps.

In our work we test this assumption with density functional theory based transport calculations of graphene bicrystals. In particular, we extend our analysis of the interplay between grain boundary structure and transport properties [2] by including mechanical strain. We compute transmission functions and current-voltage curves and compare them with tight binding calculations. Our findings suggest that the strain-induced transport gap modulation can be fully described by the response of the bulk graphene band structure towards strain.

[1] Riaz *et al.*, Nanotechnology **26**, 325202 (2015)
[2] Perera *et al.*, Phys. Rev. B **98**, 155432 (2018)

O 58: Focus Session: Electron-Phonon Interactions II

Time: Wednesday 15:00–17:15 Location: H15

Invited Talk O 58.1 Wed 15:00 H15

Towards a systematic way of treating non-adiabatic effects — •E.K.U. Gross — Max Planck Institut of Microstructure Physics, 06120 Halle, Germany

Some of the most fascinating quantum phenomena, such as the process of vision or phonon-driven superconductivity are examples of non-adiabatic effects. To treat such phenomena in a genuine first-principles way, one has to start from the full Hamiltonian of the complete system of electrons and nuclei. We employ the exact factorization [Abedi, Maitra, Gross, PRL 105, 123002 (2010)] of the full electron-nuclear wavefunction into a purely nuclear part and a many-electron wavefunction which parametrically depends on the nuclear configuration and carries the meaning of a conditional probability amplitude. The equations of motion of these wavefunctions uniquely define “exact phonons” beyond the Born-Oppenheimer approximation and the electron-phonon interaction (to all orders) in a very compact way. In addition to the exact potential energy surface there appears a Berry-type vector potential in the ionic equation of motion which gives rise to a geometric phase beyond the Born-Oppenheimer limit. We discuss how this exact geometric phase differs from the Born-Oppenheimer Berry phase, and how this difference can potentially be measured [Requist, Proetto, Gross, PRA 96, (6), 062503, (2017)]. In the time-domain, we deduce, from the exact equations of motion, a novel mixed-quantum-classical algorithm [Min, Agostini, Tavernelli, Gross, JPCL 8, 3048 (2017)] which provides a much improved (over surface hopping) description of decoherence.

O 58.2 Wed 15:30 H15

Exact factorization density functional theory of electron-phonon systems — •Ryan Requist[1], Cesar Proetto[2], and Eberhard K. U. Gross[1,3] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Centro Atomico Bariloche and Instituto Balseiro, San Carlos de Bariloche, Argentina — [3]Fritz Haber Center for Molecular Dynamics, Jerusalem, Israel

In this talk, I will discuss how to generalize density functional theory to incorporate nonadiabatic electron-phonon coupling effects. Kohn-Sham equations that yield the electronic density $n_U(\mathbf{r})$, conditional on the set of all phonon normal mode amplitudes $U = \{U_{\mathbf{q}\lambda}\}$, are coupled to the nuclear Schrödinger equation of the exact factorization scheme [1,2]. An orbital-dependent functional approximation for the nonadiabatic exchange-correlation energy is proposed. It is shown to exactly reproduce the leading-order nonadiabatic electron-phonon coupling effects, e.g. electronic velocity renormalization, in the Fröhlich model.

[1] Phil. Trans. Roy. Soc. A 372, 20130059 (2014); [2] Phys. Rev. Lett. 105, 123002 (2010)

O 58.3 Wed 15:45 H15

Superconductivity from first-principles in sodalite yttrium hydrides — •Simone Di Cataldo[1], Christoph Heil[1], Lilia Boeri[2], and Giovanni Bachelet[2] — [1]Institute of Theoretical and Computational Physics, Graz University of Technology, NAWI Graz, 8010 Graz, Austria — [2]Dipartimento di Fisica, Sapienza Università di Roma, 00185 Roma, Italy

The recent experimental discovery of the record-breaking critical superconducting temperature of 265 K in a lanthanum superhydride (LaH_{10}), following the one of 203 K in SH_3 three years ago, firmly supports hydrides as promising candidates in the search for room-temperature superconductivity.

In our work we use Density Functional Theory, together with fully anisotropic first-principles Migdal-Eliashberg theory to investigate the electronic, vibrational and superconducting properties of two yttrium hydrides (YH_6 and YH_{10}), which are closely related to the corresponding lanthanum hydrides, but have been predicted to exhibit even higher T_cs. We show that the superconducting properties are rather uniform over all phonon and electronic states, meaning that the origin of the strong electron-phonon coupling cannot be explained only in terms of the hydrogen sublattice, but is rather due to the interaction between the host atom and the whole clathrate sublattice. A comparison of the pressure behavior of the T_c of the two compounds suggests a route to lower the pressure to high T_c superconductivity.

O 58.4 Wed 16:00 H15

No superconductivity in iron polyhydrides at high pressures — •Lilia Boeri[1], Christoph Heil[2], and Giovanni Bachelet[1] — [1]Dipartimento di Fisica, Sapienza Universita' di Roma, Italy — [2]ITP-CP, Graz University of Technology, Austria

A recent experimental study [1] reported the formation of several new iron polyhydrides FeHx at pressures in the megabar range and spotted FeH5, which forms above 130 GPa, as a potential high-Tc superconductor because of an alleged layer of dense metallic hydrogen. Shortly after, two studies based on ab initio Migdal-Eliashberg theory seemed to independently confirm such a conjecture. We conversely find, on the same theoretical-numerical basis, that neither FeH5 nor its precursor, FeH3, shows any conventional superconductivity and explain why this is the case.

[1] C. Pepin et al., Science 357, 382 (2017).

O 58.5 Wed 16:15 H15

Simulation of electronic friction effects in chemical dynamics at metal surfaces: Understanding the successes and failures of ab-initio methods — •Connor Box and Reinhard J. Maurer — Department of Chemistry, University of Warwick, United Kingdom

The coupling of molecular adsorbate motion with hot electrons in a metal substrate represents a breakdown of the Born-Oppenheimer approximation with measurable consequences. An accurate theoretical description of how these hot electron effects modify the reaction dynamics of molecules on metals will be essential to utilize light-matter interaction in catalysis. The electron-phonon coupling between adsorbate vibrations and hot electrons are efficiently described in a density functional theory-based molecular dynamics with electronic friction (MDEF) approach, where electronic friction forces act on atoms within a Langevin framework. [1] Several methods have been proposed to describe electronic friction; however, more work remains to be done to provide a transferable and accurate description of experimental findings. In this talk, we present our efforts towards pushing beyond the current limitations of the MDEF method. We explore the consequences of existing approximations in MDEF calculations for the frequently studied carbon monoxide adsorbed Cu(100) and Pt(111) surfaces. [2] We systematically assess the importance of substrate motion, vibrational anharmonicity, and mode coupling in comparison with recently published many-body perturbation theory results [3] to guide future directions of method development. [1] PRL 116, 217601 (2016), [2] PRB 94, 115432 (2016), [3] PRL 120, 156804 (2018)

O 58.6 Wed 16:30 H15

Nonadiabatic effects in electron and phonon spectra of electron-doped monolayer MoS_2 from first-principles calculations — •peio garcia-goiricelaya[1,2], jon lafuente-bartolome[1,2], idoia g.gurtubay[1,2], and asier eiguren[1,2] — [1]Materia Kondentsatuaren Fisika Saila, University of the Basque Country UPV/EHU, 48080 Bilbao, Basque Country, Spain — [2]Donostia Interational Physics Center (DIPC), Paseo Manuel de

Lardizabal 4, 20018 Donostia-San Sebastián, Spain

We present a complete *ab initio* analysis of the electron-phonon interaction in the electron-doped monolayer MoS_2, a system that is attracting growing interest, specially after the discovery of gate-induced spin-locking superconductivity [1]. Also recently, intriguing renormalized band structure has been observed in this system [2], which calls into question the exact mechanism by which electron-phonon interaction is so effective. Our calculations uncover the exceptional quasiparticle band-splitting structure. Directly connected to the renormalized electron structure, we complement the study by analyzing the nonadiabatic phonon spectrum, where we predict also strong vibrational branch renormalization for some modes. These results are illustrated with the help of simplified model calculations.

[1] Ye, J.T. *et al.* Superconducting dome in a gate-tuned band insulator. *Science* **338**, 1193-1196 (2012).

[2] Kang, M. *et al.* Holstein polaron in a valley-degenerate two-dimensional semiconductor. *Nature Materials* **17**, 676-680 (2018).

O 58.7 Wed 16:45 H15

Phonon renormalization in ab-initio-based lattice models — •Jan Berges[1], Malte Roesner[2,3], Erik van Loon[1], and Tim Wehling[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Department of Physics and Astronomy, University of Southern California, Los Angeles, USA — [3]Center for Computational Quantum Physics, Flatiron Institute, New York, USA

Phonons play a major role in the understanding of phenomena such as superconductivity, periodic lattice distortions, magnetostriction, thermo- and piezoelectrics. Yet, despite the success of *density-functional perturbation theory* (DFPT), their ab-initio calculation remains challenging for structurally complex and strongly interacting systems. To address these problems, we introduce a computational scheme based on material-realistic quantum lattice models, that combine the efficiency of a lattice model with an ab-initio input and the freedom to choose different levels of approximation to treat electron-electron interactions. In our scheme, all parameters are derived ab initio, using the *constrained* methods cRPA and cDFPT [Nomura, Arita: Phys. Rev. B **92**, 245108 (2015)]. In the presented work, we apply our scheme to the metallic *transition-metal dichalcogenides* (TMDCs), prominent showplace for coexisting many-body instabilities. First, we demonstrate that the fully renormalized ab-initio results are exactly reproduced by our model if we solve it at the level of the *random-phase approximation* (RPA). Then we study the influence of charge doping and hybridization with substrates.

O 58.8 Wed 17:00 H15

Efficient calculation electron-phonon related problems thought Helmholtz Fermi Surface harmonics (HFSH). — Jon Lafuente-Bartolome[1,2], Idoia G. Gurtubay[1,2], and •Asier Eiguren[1,2] — [1]Condensed Matter Physics Dept. Uni. Basque Country (UPV/EHU), Spain — [2]Donostia International Physics Center (DIPC), San Sebastian, Spain

In a metals, the details ls of the Fermi surface and the magnitude of the matrix elements connecting different points defined on it determine most of the transport properties, which are limited by the electron-phonon coupling and the scattering by impurities. While typically the calculation of an anisotropic Fermi surface realted physical property requires the consideration several thousand points on the surface, say in an impurity or Boltzmann transport problem, the Helmholtz Fermi Surface harmonics (HFSH) technique allows us to accurately treat these problems considering few elements of the HFSH set. Here we introduce the recent developments in this direction, including the symmetry treatment and derived selection rules, and a representative benchmarking list of examples illustrating the potential of this method.

O 59: 2D Materials III: Nanomembranes, hBN, and Particle Interactions

Time: Wednesday 15:00–17:30 Location: H16

O 59.1 Wed 15:00 H16

Molecular dynamics investigation of Young's moduli of carbon nanomembranes (CNMs) — •Julian Ehrens[1], Florian Gayk[1], Tjark Heitmann[2], Patrick Vorndamme[1], and Jürgen Schnack[1] — [1]Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany — [2]Osnabrück University, Neuer Graben/Schloss, 49074 Osnabrück, Germany

Nanometer thin carbon nanomembranes (CNMs) are made by electron-induced crosslinking of aromatic self-assembled monolayers (SAMs) [1]. Their supposedly irregular internal structure can not be adequately investigated by X-ray diffraction, but by a characterization through physical quantities like solvent permeability and Young's modulus. In order to propose possible structures of these membranes we investigate various initial configurations of the SAM and excitation processes that mimic the impact of the radiation together with their impact on the Young's modulus. For all calculations classical molecular dynamics as implemented in LAMMPS is employed. Preliminary studies have been made in benchmarking the accuracy of several classical carbon potentials concerning Young's moduli [2]. We discuss two methods to obtain the moduli: application of homogeneous scaling and directional strain to the monolayer.

[1] Turchanin et al., Progress in Surface Science, Volume 87, Issues 5-8, May-August 2012, Pages 108-162

[2] Gayk et al., Physica E: Low-dimensional Systems and Nanostructures, Volume 99, May 2018, Pages 215-219

O 59.2 Wed 15:15 H16

Preparation of Carbon Nanomembranes from SAMs with carboxylic binding groups on silver substrates — •Christof Neumann[1], Monika Szwed[2], Martha Frey[1], Zian Tang[1], Piotr Cyganik[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland

The electron irradiation induced synthesis of Carbon Nanomembranes (CNMs) from aromatic thiol-based self-assembled monolayers (SAM) is a well-established method to form molecular thin nanosheets [1]. These molecular 2D materials can be prepared with tunable properties and therefore they find a variety of applications in nanotechnology ranging from ultrafiltration to nanobiosensors [2]. Here we study the conversion of SAMs with aromatic-aliphatic backbones and carboxylic head groups [3,4] into CNMs on silver substrates. To this end, we employ high-resolution X-ray photoelectron spectroscopy, low-energy electron diffraction, atomic force microscopy and scanning electron microscopy. We find a clear correlation between the length of the aliphatic chain in the precursor molecules and the properties of the formed CNMs. Moreover, we compare these results with the formation of CNMs from thiol-based molecular counter partners. [1] P. Angelova, A. Turchanin et al., ACS Nano 7, 6489-6497 (2013) [2] A. Turchanin, A. Gölzhäuser, Adv. Mater. 28, 6075-6103 (2016) [3] A. Krzykawska, P. Cyganik et al., Chem. Comm. 53,5748-5751 (2017) [4] A. Krzykawska, P. Cyganik et al., J. Phys. Chem. C 122, 919-928 (2018)

Invited Talk O 59.3 Wed 15:30 H16

Carbon Nanomembranes: Preparation, Properties, and Applications — •Xianghui Zhang — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Carbon Nanomembranes (CNMs) are two-dimensional sheets with tailored physical and chemical properties. I will first give an overview of the preparation of CNMs and their mechanical, optical and electronic characteristics. Then I will present several recent findings on the structure of CNMs using surface-enhanced Raman spectroscopy and scanning probe microscopy, which make CNMs of interest for applications in energy storage and membrane separations. Finally, I will show the realization of all-carbon capacitors composed of CNMs as dielectrics sandwiched between two graphene electrodes, and will further address how the CNM allows for a fast yet selective transport of water and helium through sub-nanometer channels.

[1] A. Turchanin, A. Gölzhäuser, Adv. Mater. 28, 6075 (2016) [2] X. Zhang, M. Mainka, et al., Langmuir, 34, 2692 (2018) [3] X. Zhang, E. Marschewski, et al., ACS Nano, 12, 10301 (2018) [4] Y. Yang, P. Dementyev, et al., ACS Nano, 2018, 12, 4695 (2018)

O 59.4 Wed 16:00 H16

Au-Rh surface alloy for tuning the nanomesh structure of

h-BN — •Krisztián Palotás[1,2,3], László Óvári[3], Gábor Vári[3], Richárd Gubó[3], Arnold Farkas[3], János Kiss[3], András Berkó[3], and Zoltán Kónya[3] — [1]Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]University of Szeged, Szeged, Hungary

Hexagonal boron nitride (h-BN) monolayer on the Rh(111) substrate has a periodically corrugated "nanomesh" structure. On the other hand, h-BN layer on a clean Au(111) substrate is atomically flat. By forming surface alloys of Au-Rh in different compositions on a Rh(111) substrate, we report on the gradual tunability of the nanomesh morphology of h-BN [1], which can be useful for various nanopatterning applications. Increasing the Au amount in the surface alloy results in reduced pore diameter and corrugation of the h-BN layer [1]. The experimental findings are confirmed by density functional theory calculations: The energetically preferred ordered (2x1) Au-Rh surface alloy [2,3] is reconstructed, and Rh is accummulated below the pore of h-BN.

References: [1] R. Gubó et al., Phys. Chem. Chem. Phys. 20, 15473 (2018). [2] L. Óvári et al., Phys. Chem. Chem. Phys. 18, 25230 (2016). [3] K. Palotás et al., J. Phys. Chem. C 122, 22435 (2018).

O 59.5 Wed 16:15 H16

Real-time investigation of the growth of hexagonal boron nitride on the Ni(111) surface — •Miriam Raths[1,2], Janina Felter[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology, Germany

The 2D material hexagonal boron nitride (hBN) has attracted strongest interest recently due to its specific structural and electronic properties. In this study, we aim for a deeper understanding of its nucleation and growth behavior, as this is necessary to produce high quality layers of hBN.

The growth of hBN on the Ni(111) surface depends strongly on the preparation of the substrate before deposition. In our study, we have used two different cleaning methods for the substrate resulting in different defects densities. In both cases, the growth of hBN was imaged in-situ and in real time by means of LEEM. Four different structures were found on the surface: (1) A commensurate and (2) a rotated hBN monolayer structure, the latter with various azimuthal rotation angles, as well as two bilayer structures consisting of either (3) two rotated or (4) one commensurate and one rotated layer of hBN. While the formation of all of these structures was observed on the Ni(111) surface with low defect density, at higher defect density only the two monolayer phases were found. For both growth experiments, we present a detailed analysis of (bright and dark field) LEEM and μLEED data.

O 59.6 Wed 16:30 H16

How Graphene and Hexagonal Boron Nitride Get Electrified in Water? — •Benoit Grosjean, Marie-Laure Bocquet, and Rodolphe Vuilleumier — PASTEUR, Département de chimie, École normale supérieure, PSL University, Sorbonne Université, CNRS, 75005, Paris, France

The recent emergence of nanofluidics has highlighted the exceptional properties of graphene and its boron-nitride counterpart (hBN) as confining materials for water and ion transport. Surprinsingly ionic transport experiments have unveiled a large electrification of the water-BN surfaces, with a contrasting response for its water-carbon homologue. This charging was conjectured to originate in the differential hydroxide adsorption on the 2D materials, but the challenge of simulating this elusive anion has precluded a proper explanation up to now. We report free energy calculations based on ab initio molecular dynamics simulations of a hydroxide in water near graphene and hBN layers. Our results(1) disclose that both surfaces electrify by hydroxide adsorption via different mechanisms. OH- shows strong chemisorption on hBN, but only weak physisorption on graphene. Interestingly OH- is shown to keep a fast lateral interfacial mobility while physisorbed. Taking into account the resulting large ionic surface mobility, an analytical transport model allows to reproduce quantitatively the experimental data. Our results offer new foundations for the chemical reactivity of carbon and BN materials in water and suggest new perspectives for advanced membrane technologies for water purification and energy harvesting.

(1) B. Grosjean, M.-L. Bocquet and R. Vuilleumier, Submitted, 2018

O 59.7 Wed 16:45 H16

Charge exchange between highly charged ions and 2D materials — •Sascha Creutzburg[1,2], Janine Schwestka[3], Mukesh K. Tripathi[4], Heena Inani[4], René Heller[1], Nico Klingner[1], Anna Niggas[3], Tibor Lehnert[5], Robert Leiter[5], Roland Kozubek[6], Stefan Facsko[1], Ute Kaiser[5], Jani Kotakoski[4], Marika Schleberger[6], Friedrich Aumayr[3], and Richard A. Wilhelm[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Ion Beam Center, Dresden, Germany — [2]TU Dresden, Germany — [3]TU Wien, Institute of Applied Physics, Vienna, Austria — [4]University Vienna, Faculty of Physics, Austria — [5]Ulm University, Central Facility of Electron Microscopy, Ulm, Germany — [6]University Duisburg-Essen, Faculty of Physics and CENIDE, Duisburg, Germany

The neutralisation of ions due to their interaction with matter deals with fundamental aspects of ion-solid interaction, e.g.: How does the kinetic energy loss depend on the charge exchange? In order to investigate the neutralisation behaviour, classical ion beam foil experiments were performed using ultimately thin 2D materials as target. Because of their low thickness, an ion with a sufficiently high incident charge state does not reach charge equilibrium, which enables the measurement of the non-equilibrium exit charge state distribution. The influence of target material properties on the charge exchange is investigated for 2D materials consisting of graphene, MoS_2 and hBN, which show different band gap energies between 0 and 6 eV, conductance properties (metallic, semi-conducting and insulating) and layer structures.

O 59.8 Wed 17:00 H16

Unraveling energy-loss processes of low energy heavy ions in 2D materials — •Richard A. Wilhelm[1,2] and Pedro L. Grande[3] — [1]TU Wien, Institute of Applied Physics, Austria — [2]HZDR, Institute of Ion Beam Physics and Materials Research, Germany — [3]Federal University of Rio Grande so Sul, Institute of Physics, Ion Implantation Laboratory, Brazil

In order to use ion beams for defect engineering of 2D materials, a model for energy deposition is needed, which takes the ion charge state and charge exchange into account. In the first monolayers of a material impinging keV ions capture electrons and reduce their charge state until charge equilibrium is reached in less than 10 fs (about 1 nm).

We present here a new model for charge state and charge exchange dependent ion stopping force calculation, which shows that heavy ions in charge states greater than 1 deposit a substantially larger amount of their kinetic energy in a 2D material than predicted by standard tools as e.g. SRIM. This holds true for electronic and nuclear energy losses, whereas especially the latter causes sputtering and therefore structural defects.

Our model relies an a time-dependent scattering potential, which changes due to charge exchange and electronic de-excitation of the projectile during collision. We compare our model results with experimental values determined by heavy highly charged ion transmission through freestanding single layer graphene and find very good agreement in energy loss, charge state distributions, and scattering angle-dependent charge exchange.

O 59.9 Wed 17:15 H16

Characterization of interlayer forces in 2D heterostructures using neutral atom scattering — •Amjad Al Taleb[1,2], Gloria Anemone[1], Rodolfo Miranda[1,2,3,4], and Daniel Farías[1,3,4] — [1]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain — [2]Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nanociencia), Madrid, Spain — [3]Instituto 'Nicolás Cabrera', Madrid, Spain — [4]Condensed Matter Physics Center (IFIMAC), Madrid, Spain

We show that neutral atom scattering is suitable to determine the coupling strength between a two-dimensional (2D) material and the underlying substrate. This information can be obtained from the thermal attenuation of the specular intensity, as well as from angular distributions of He and Ne atoms in the low incident energy (20-50 meV) regime. For graphene (Gr) grown on several metal substrates, there is a direct correlation between the slope of thermal attenuation measurements and the Gr-substrate coupling strength obtained from surface phonons measurements. In addition, Ne scattering presents a broad, classical angular distribution when the Gr-substrate coupling is weak, like in Gr/Ir(111), whereas sharp diffraction features are observed for strongly interacting systems, like Gr/Ru(0001). The influence of the moiré superstructures on this simple picture is also discussed. This superstructures induces a splitting of the flexural mode of Gr in addition of additional phonon dispersion lines as a result of Umklapp scattering. We show evidence of the localization of the phonon modes from the difference in their thermal attenuation behaviors.

O 60: Organic Molecules on Inorganic Substrates IV: Electronic Properties, Excitations, Dynamics

Time: Wednesday 15:00–17:30 Location: H24

O 60.1 Wed 15:00 H24

Quantum size oscillations of oligoacene gaps adsorbed on Au(111) — •Richard Korytár — Charles University, Prague, Czech Republic

For gas phase oligoacenes, our recent theoretical work suggests a possibility for oscillations of the excitation gaps with the length of the molecule. In view of the recent experimental progress of on-surface synthesis, we employ the density functional theory to investigate here the fate of these oscillations for oligoacenes adsorbed on a Au(111) surface. Since the long range-nature of the Coulomb interaction is removed on metallic substrates due to screening, correlation effects are weaker and the tendency towards oscillatory behavior is enhanced.

O 60.2 Wed 15:15 H24

Excited state dynamics and transient band structure changes in molecular thin films — •Sebastian Hedwig[1], Sebastian Emmerich[1], Johannes Stöckl[1], Benito Arnoldi[1], Mirko Cinchetti[2], Stefan Mathias[3], Benjamin Stadtmüller[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany — [3]Georg-August-Universität Göttingen, Göttingen 37077, Germany

The future success of organic materials in optoelectronic applications relies on our ability to understand and optimize their optical and transport properties. Despite their common origin – the electronic band structure – their interplay in organic materials is far from being understood. In this context, we recently employed time-resolved photoelectron spectroscopy with fs-pulsed XUV-radiation to reveal a direct correlation between the excited state dynamics of a thin C_{60} film on Ag(111) and a transient inhomogeneous broadening of the entire occupied valence states upon optical excitation. Here, we extend our recent study to different C_{60} coverages between one and ten monolayers to determine the role of the Ag(111) substrate for the timescale and the magnitude of the transient band structure broadening. Moreover, additional time- and momentum resolved photoemission data will allow us to reveal possible transient changes in the molecular band dispersion of the C_{60} films upon optical excitation with visible light.

O 60.3 Wed 15:30 H24

Excited Electron Dynamics in Thiophene-based Polymers — •Tobias Reiker[1], Carsten Winter[1], Deb Kumar Bhowmick[1], Nils Fabian Kleimeier[1], Zitong Liu[2], Deqing Zhang[2], and Helmut Zacharias[1] — [1]Center For Soft Nanoscience, Westfälische Wilhelms-Universität Münster — [2]Institute of Chemistry, Chinese Academy of Science, Beijing, China

An internal donor-acceptor system is formed by thiophene polymers coupled with pyrrole chains. Different alkyl side chains can improve the interchain packing and affect the backbone conformation, further they can directly influence the charge transporting behavior. Although OFETs and organic photovoltaic cells have been already successfully utilized, the exact internal dynamics of the system are still under investigation. In this presentation we show the results of a time-dependent photoemission study on the thiophene polymers PDPP4T and DTT on a Si(100) substrate. Occupied electronic levels were analyzed with UPS. The fundamental and third harmonics of a Ti:Sapphire laser system with a time-of-flight spectrometer are utilized for static 2PPE to determine the energetic positions of high lying occupied and intermediate unoccupied states. Dynamic 2PPE is then used to study the electron dynamics of the intermediate states directly in the time domain and shows three distinct electronic lifetimes. Depending on the electron kinetic energy lifetimes of a few hundred femtoseconds, up to 3 ps and a slow channel around 15 ps are observed. After annealing at 180°C an unoccupied state at an exitation energy of 0.40 eV loses its long-lived component.

O 60.4 Wed 15:45 H24

Single photon plasmonic emission from STM-induced quantum dots — •Christopher C. Leon[1], Dimas G. de Oteyza[2,3,4], Anna Rosławska[1], Pablo Merino[1,5], Abhishek Grewal[1], Klaus Kuhnke[1], and Klaus Kern[1,6] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany. — [2]Donostia International Physics Center, San Sebastian, Spain. — [3]Centro de Fisica de Materiales, CSIC-UPV/EHU, San Sebastian, Spain. — [4]Ikerbasque, Basque Foundation for Science, Bilbao, Spain. — [5]present address: Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain. — [6]Institut de Physique, École Polytechnique Fédérale de Lausanne, Switzerland.

A hallmark of quantum control is the ability to make photons at the nanoscale whose temporal features are distinct from classical light sources. Through scanning tunneling microscopy induced luminescence (STML) we are able to generate plasmonic light originating from inelastic tunneling processes that occur in few-nanometer thick molecular films of C_{60} deposited on Ag(111). This light is antibunched with a $1/e$ recovery time of less than one nanosecond, as shown through Hanbury Brown and Twiss photon intensity interferometry. These phenomena are attributed to a Coulomb blockade that occurs when tunneling electrons are forced to hop through a discrete quantum state that is created from the strong electric field of the tip and its confinement effects. The spatial extent of this state can be varied by adjusting the degree of band bending through the sample.

O 60.5 Wed 16:00 H24

Adsorption, Orientation and Reactivity of Phenylphosphonic Acid on Rutile TiO_2(110) — •Julia Köbl, Daniel Wechsler, Elmar Kataev, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie 2, Universität Erlangen Nürnberg, Egerlandstraße 3, D-91058

To fully understand organic electronic devices, such as dye-sensitized solar cells, it is necessary to understand the interactions of organic molecules with oxide substrates at the atomic level. To facilitate this understanding, we have studied the adsorption and reactivity of phenylphosphonic acid on TiO_2(110) - 1 × 1. Using Synchrotron Radiation Photoelectron Spectroscopy (SRPES) and Near-Edge X-ray Absorption Fine-Structure Spectroscopy (NEXAFS) we have studied the thermal stability and bonding mechanism of phenylphosphonic acid at temperatures up to 900 K. High-resolution O 1s spectra exhibit three distinct oxygen species on the surface, and NEXAFS C K-edge measurements reveal a mostly upright standing adsorption geometry at all temperatures. Supported by the DFG through FOR 1878 (funCOS).

O 60.6 Wed 16:15 H24

Adsorption of phosphonate functionalized porphyrin molecules on TiO2(110) surfaces — Cynthia Fernandez[1], Daniel Weschler[2], Hans-Peter Steinrück[2], Ole Lytken[2], and •Federico Williams[1,2] — [1]Departamento de Química Inorgánica, Analítica y Química Física, Universidad de Buenos Aires, Argentina — [2]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Erlangen, Germany

Solar energy technologies including dye-sensitized solar cells and water-splitting photoelectrochemical cells are constructed linking chromophores to semiconductor surfaces. Promising systems are based on porphyrins bonded to TiO2 surfaces. One of the critical factors affecting device performance is the molecular adsorption geometry. Therefore, fundamental research studying the interaction of porphyrins with TiO2 surfaces is important. Here, we studied the bonding and adsorption geometry of tetraphenyl porphyrin molecules containing one or four phosphonate groups. The investigation was carried out by means of synchrotron radiation X-ray photoelectron spectroscopy (XPS) and near edge X-ray absorption fine structure (NEXAFS) measurements. Our results show that the number of linker groups have a great influence on the adsorption geometry. Molecules with one phosphonate group adsorb with the macrocycle tilted away from the surface whereas molecules with four phosphonate groups adsorb with the macrocycle close to the surface. This is an important finding for the design of dye-sensitized solar and photoelectrochemical cells. This project is supported by the DFG through FOR 1878 (funCOS).

O 60.7 Wed 16:30 H24

X-Ray Small Angle In-Situ Study of Porphyrin Adsorption on Stabilized Rutil Surfaces — •Klaus Götz, Annemarie Pfnür, and Tobias Unruh — Institute for Crystallography and Structural Physics, Erlangen, Germany

Dye sensitized solar cells (DSSCs) based on TiO2 have been studied as an easy to produce, low-cost alternative to classical semiconductor solar cells with recent efficiencies of up to 13% for a long time [1][2]. We synthesized tunable titania nanoparticles with a diameter of 2-3 nm that are stabilized by oleic acid. Special emphasis of our work is focused on the exchange process of the oleic acid with porphyrins designed for a particular application.

This process is studied using a variation of different x-ray small angle scattering techniques. One method is the combination of small angle x-ray and neutron scattering (SAXS and SANS) experiments. These are well suited to study core/shell systems because of the different scattering lengths for x-rays and neutrons. On the other hand x-ray reflectivity measurements can be used to study layered systems on flat substrates. This offers the possibility to study the exchange of oleic acid with porphyrins on TiO2 Wafers as a test system. In the talk an overview over the different techniques will be given. Furthermore their usage in the characterization of the morphology of the produced particles and the ligand exchange from oleic acid to porphyrins will be presented.

[1] O'Regan & Grätzel; Nature 353, 737-740 (1991)
[2] Matthew S. et al.; Nat. Chem. 6; 242-247 (2014)

O 60.8 Wed 16:45 H24

Molecular dynamics simulation of transport and nucleation of conjugated organic molecules on inorganic surfaces — •Mila Miletic[1,3], Karol Palczynski[1], Matheus R. Jacobs[3], Ana M. Valencia[3], Caterina Cocchi[3], and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, Freiburg, Germany — [3]Physics Department, Humboldt-Universität zu Berlin, Berlin, Germany

We analyze the influence of polarity on the surface transport of single conjugated organic molecules on the inorganic $(10\bar{1}0)$ zinc oxide surface by all-atom molecular dynamics simulations at room temperature and above. In particular, we study the effects of partial fluorination of the *para*-sexiphenyl *p*-6P molecule with chemical modifications of one head group *p*-6PF2 or both head and tail *p*-6PF4. We show that quantum and classical simulations both find consistent and highly distinct dipole moments for the three studied molecules. The diffusion of both p-6P and its fluorinated derivatives is Arrhenius-like, governed by thermally activated energy barrier crossings. Also, *p*-6P has a lower diffusion energy barrier compared to its fluorinated derivatives in the nonpolar direction of the anisotropic surface, while the barrier in the polar direction is about 20 kJ/mol higher. This rather unexpected behaviour is governed by a subtle balance of electrostatic attractive and repulsive molecule-substrate interactions as well as substantial entropic contributions coming from orientational and internal molecular degrees of freedom. Our findings can help to control the kinetics of nucleation and growth in the future design of hybrid organic-inorganic interfaces.

O 60.9 Wed 17:00 H24

Tuning the adsorption geometry of cyano-substituted porphyrins on bulk insulators — •Min-Ken Li, Mirunalini Devarajulu, Jia Liu, Maximilian Ammon, and Sabine Maier — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

The realization of molecular-based devices requires the adsorption of molecular building blocks on insulating substrates to preserve their original functionality. Therefore, organic molecules on insulating surfaces have been attracting more attention recently. Porphyrins are of particular interest because they are robust, and their adsorption and electronic properties can be changed by chelation of a metal ion or substitution of anchor groups on the macrocycle; both tune the interplay between intermolecular and molecule-surface interactions.[1] Here, we report on the adsorption geometry and self-assembly of cyano-substituted porphyrin derivatives on bulk KBr(001), MgO(001), and Au(111) surfaces using non-contact atomic force microscopy and scanning tunneling microscopy featuring sub-molecular resolution at low temperature. We demonstrate that the adsorption geometry of mono-cyano-substituted porphyrin derivatives can be tuned by functional side groups from nearly up-right standing to flat lying.[2] Moreover, we will discuss the influence of the central metal ion, the number of cyano-groups as well as the substrate on the adsorption geometry and the structure formation of self-assemblies.

[1] J.M.Gottfried, Surf. Sci. Rep., 2015, 70, 3, 259-379
[2] S. Maier, et al. Small, 2008, 4, 1115-1118

O 60.10 Wed 17:15 H24

Metalation and Polymerization of 5,5'-Dibromosalophene on Co-intercalated Graphene — •Julia Goedecke[1], Micha Elsebach[1], Michael Rohde[1], Emil Sierda[1,2], Maciej Bazarnik[1,2], and Roland Wiesendanger[1] — [1]Dept. Physics, University of Hamburg, D-20355 Hamburg, Germany — [2]Institute of Physics, Poznan University of Technology, Piotrowo 3, 60-965 Poznan, Poland

Salophene complexes are suitable for molecular spintronic applications due to their chemical structure and electronic and magnetic properties. In previous work of Bazarnik et al. a concept for an all-spin molecular device with Co-salophenes on Au(111) has already been presented[1]. Using STM and STS we will show that such an approach can also be realized on Co-intercaleted graphene on Ir(111), a much more inert surface that limits the hybridization with the complexes and does not show a Kondo-effect, as is the case with Co-Salophenes on Au(111)[2]. For this purpose 5,5'-Dibromosalophenes were metallized *in situ* via surface reaction in UHV with different transition metals, namely with Co, Cr and Fe. Furthermore, we will show that these *in situ* produced Salophene complexes can be polymerized on the graphene surface via Ullmann like reaction[3] and therefore are suitable for a molecular spintronic device.

[1] M. Bazarnik et al., Nano Lett. 16, 577 (2016)
[2] A. DiLullo et al., Nano Lett. 12, 3174 (2012)
[3] F. Ullmann et al., Chemische Berichte, 34 (2): 2174 (1901)

O 61: Semiconductor Surfaces: Adsorption and Reactivity

Time: Wednesday 15:00–17:30 Location: H25

O 61.1 Wed 15:00 H25

Atomic structure of As-modified Si(100) surfaces prepared in MOCVD ambient — •Agnieszka Paszuk[1], Oleksandr Romanyuk[2], Oliver Supplie[1], Manali Nandy[1], Peter Kleinschmidt[1], and Thomas Hannappel[1] — [1]Institute for Physics, University of Technology, Ilmenau, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

For highly efficient III-V-on-Si tandem solar cells it is crucial to avoid defects known as antiphase boundaries at the III-V/Si interface by preparing the Si(100) surface with double-layer (DL) steps. While preparation of the DL-stepped Si(100) surfaces in As-rich metalorganic chemical vapor deposition (MOCVD) ambience has been investigated, their surface structure is still not fully understood. Here, the DL-stepped Si(100) surfaces are prepared in As-rich MOCVD ambience and the entire process is monitored by optical *in situ* spectroscopy. The Si:As surfaces are investigated by surface-sensitive techniques in ultra-high vacuum. With scanning tunneling microscopy (STM), we observe different Si:As surface structures in dependence on the substrate miscut and preparation routes. The low-offcut Si(100):As surfaces exhibit evenly spaced, atomically flat terraces with a random distribution of darker and brighter areas, which stem from a different local electronic structure. STM scans of vicinal Si(100):As surfaces show zig-zag chains and asymmetrical protrusions. Density functional theory calculations predict that, in H_2 ambient, the commonly assumed As-As dimer termination on top of Si(100) is not energetically favorable and the surface structure strongly depends on the H and As chemical potentials.

O 61.2 Wed 15:15 H25

The impact of Al on defects introduced during GaP nucleation on Si(100) 2° substrate by MOCVD — •Manali Nandy, Agnieszka Paszuk, Christian Koppka, Oliver Supplie, Peter Kleinschmidt, and Thomas Hannappel — Institute for Physics, University of Technology, Ilmenau, Germany

The performance of III-V-on-Si multi-junction solar cells is still limited by a high density of defects at the GaP/Si heterointerface and in the III-V buffer. Here, the GaP buffers are grown on Si(100)2° substrates by metalorganic chemical vapor deposition in Al-free (as a reference) or in Al-containing reactors. In the latter one, Al was supplied either directly during the GaP nucleation from the TMAl precursor or indirectly from Al residuals present in the reactor from previous processes. Defects in the GaP buffers are investigated by electron channeling contrast imaging (ECCI). The GaP buffers grown on GaP nucleation in the Al-free reactor exhibit short misfit dislocations (MDs) and a high density of stacking faults (SFs). In contrast, in the GaP buffers prepared in the Al-containing reactor, the MDs are longer and the density of SFs is lower. Long MDs reduce the lattice strain which results in a smoother GaP surface morphology compared to the GaP buffers with short MDs. GaP buffers grown on modified GaP nucleation layer with Al exhibit even longer MDs, lower density of threading dislocations and very smooth surface morphology. Possibly due to the lower mobility of Al compared to Ga, the surface coverage during the nucleation is improved, which further may affect the crystal quality in the GaP buffer [1].[1] A. C. Lin et al., J. Vac. Sci. Tech. B 29, 3, (2011).

O 61.3 Wed 15:30 H25

Reduction of hydrogen out-effusion by using dense silicon nitride as capping layer — •sahar Jafari — Anhalt University of applied sciences, Köthen, Germany

The dependence of hydrogen effusion out of the a-SiNx:H on its film composition and the form of hydrogen bonds was experimentally studied by using effusion measurement system. Two hydrogen evolution peaks at high and low temperatures were observed but at different temperatures while the sample was heated up to 1000 °C in a constant heat rate (20 °C/min). Regarding the N/Si values revealed from X-ray photo-electron spectroscopy, the increase of N content in SiNx shifts the hydrogen effusion peak to higher temperatures at about 900 °C. It*s assumed that the N-rich silicon nitride can act as a proper capping layer during the contact-firing process (about 800 °C) to reduce the loss of hydrogen. We have confirmed the impact of composition and remained defects at the interface of Si/SiNx and propose an optimized passivation with a stacking structure. Finally, the experimentally observed hydrogen effusion peak has been confirmed by theoretical FEM simulations of Fick*s law.

O 61.4 Wed 15:45 H25

Analysis of the Catalytic Activation of CO_2 by Artificial Intelligence Studies and Extensive DFT Calculations — •Aliaksei Mazheika[1], Yanggang Wang[1,2], Luca Ghiringhelli[1], Sergey V. Levchenko[3,1,4], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]University of Shenzhen, Shenzhen, CN — [3]Skolkovo Innovation Center, Moscow, RU — [4]NUST MISIS, Moscow, RU

Using artificial intelligence (AI) trained on *ab initio* data, we develop a strategy for the rational design of catalytic materials for converting CO_2 to fuels and other useful chemicals. Specifically, we employ the subgroup discovery [1] and sure independence screening and sparsifying operator (SISSO) [2]. For oxide surfaces the results reveal that an electron transfer to the π^* antibonding orbital of the adsorbed molecule and the associated bending of the initially linear O-C-O, previously proposed as indicator of activation [3], are insufficient to account for the good catalytic performance. Instead, our AI model identifies the common feature of a group of experimentally studied oxide catalysts in the binding of one molecular O atom to a surface cation, which results in a strong elongation and therefore weakening of the molecular C-O bond. This suggests to use the C-O bond elongation as an indicator of CO_2 activation. Based on these findings, we propose a set of new promising catalysts for CO_2 conversion, and a recipe to find more.
[1] M. Boley *et al.*, Data Min. Knowl. Disc. **31**, 1391 (2017).
[2] R. Ouyang *et al.*, Phys. Rev. M **2**, 083802 (2018).
[3] H.-J. Freund and M. W. Roberts, Surf. Sci. Rep. **25**, 225 (1996).

O 61.5 Wed 16:00 H25

Mechanisms in Photocatalytic Hydrogen Evolution — •Martin Tschurl, Constantin A. Walenta, Sebastian L. Kollmannsberger, Carla Courtois, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstraße 4, 85748 Garching, Germany

Sustainable energy production and storage is considered one of the major challenges of the future, due to the impact of global warming aggravated by burning fossil fuels. One promising technology to meet this challenge is photocatalysis. It is inspired by the idea to use sunlight for the generation of renewable fuels such as hydrogen. State-of-the-art materials often comprise co-catalyst loaded semiconductors, but these systems are still limited in efficiency. The development of more powerful catalysts may have been hindered by a lack of insights on a molecular scale, as the exact mechanistic details are so far surprisingly little understood. In this talk, detailed mechanisms of the hydrogen evolution on platinum-loaded titania are discussed from a surface science perspective. Different mechanist models to explain hydrogen evolution are discussed and compared with each other.

O 61.6 Wed 16:15 H25

Temperature Influence in the Photocatalysis of Pt-Loaded Titania (110) — •Carla Courtois, Constantin A. Walenta, Sebastian L. Kollmannsberger, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstraße 4, 85748 Garching, Germany

We show the influence of temperature for the photocatalytic alcohol conversion on an n-type semiconductor single crystal surface. The focus lies on a comparison between different alcohols as reactants on a Pt-loaded titania catalyst. The photooxidation mechanisms proceed via a direct hole transfer to the adsorbed alcohol molecules. The outcome of the photochemical reactions is strongly governed by the thermal adsorption/desorption properties of the involved molecules. Thus, the overall outcome can be controlled by the judicious choice of the reaction conditions.

O 61.7 Wed 16:30 H25

Electronic and Field Induced Manipulation of Diethyl Ether on Si(001) — •Tamam Bohamud[1], Alexa Adamkiewicz[1], Marcel Reutzel[1], Michael Dürr[1,2], and Ulrich Höfer[1] — [1]Philipps-Universität, 35037 Marburg — [2]Justus-Liebig-Universität Giessen, 35392 Giessen

Scanning tunneling microscopy is an effective tool to manipulate single atoms and molecules on surfaces. Typical excitation processes involved are direct electronic excitation or vibrational excitation via inelastic tunneling. Here we show for diethyl ether fragments on Si(001) that, depending on the tunneling bias, both direct excitation as well as field-induced hopping of the molecular fragments can be observed.

Adsorption of diethyl ether on Si(001) leads to covalently bound ethoxy and ethyl entities on the surface[1]. At room temperature, tip-induced hopping of the ethyl entity on one dimer is observed at relatively low tunneling bias. For this process, no dependence on the tunneling current is observed. On the other hand, for the same parameters but at 50 K surface temperature, no such tip-induced hopping is observed at all. We interpret these experimental results in terms of a field-assisted, thermally activated hopping process. At increased bias voltage, hopping events along the dimer rows were also observed. For this process, a linear dependence of the hopping rate on the tunneling current indicates a direct electronic excitation as origin of the tip-induced hopping process.
[1] M. Reutzel et al., J. Phys. Chem. C. 119, 6018(2015).

O 61.8 Wed 16:45 H25

Quantum Chemical Investigations of Water on Tungsten Trioxide — •Thomas Teusch and Thorsten Klüner — Carl von Ossietzky University Oldenburg, Germany

Tungsten trioxide (WO_3) is a promising material for photoanodes, due to its many advantages like the narrower band gap compared to TiO_2, which allows for absorption of a large proportion of the solar spectrum. Furthermore, the deep valence band position makes the water oxidation thermodynamically easier and the high electrical conductivity leads to good electron transport properties [1]. We try to understand the involved mechanism in the water oxidation process on an atomistic level. To achieve this, we use quantum mechanical calculations with periodic boundary conditions in terms of hybrid DFT and multiconfigurational methods in terms of complete active space-SCF [2,3]. The latter allows an insight into specific excited states. In this work, we present results of the interaction of WO_3(001) with all species occurring in water splitting. In addition, we investigate the oxidation process itself by studying both ground and excited charge transfer states with embedded cluster models. These results provide a molecular view into the water oxidation process and can also be used for high-precision wave-packet quantum dynamics which will allow for new time-resolved insights.

[1] S. Corby, et al., J. Am. Chem. Soc., 2018, 140, 16168-16177 [2] R. Dovesi, et al., Int. J. Quantum Chem. A, 2014, 114, 1287-1317. [3] F. Neese Wiley Interdiscip. Rev.: Comput. Mol. Sci., 2012, 2, 73-78.

O 61.9 Wed 17:00 H25

Proton transfers at dopamine-functionalized TiO2 interface — •Costanza Ronchi[1], Daniele Selli[1], Waranyu Pipornpong[2], and Cristiana Di Valentin[1] — [1]Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, via R. Cozzi 55, I-20125 Milano, Italy — [2]Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

Despite the many successful synthesis and applications of dopamine-functionalized TiO2 nanohybrids,[1],[2], there is not yet an atomistic understanding of the interaction of this 1,2-dihydroxybenzene derivative ligand with the titanium dioxide surfaces. In this work, based on a wide set of dispersion-corrected hybrid density functional theory (DFT) calculations and on density functional tight binding (DFTB) molecular dynamics simulations, we present a detailed study of the adsorption modes, patterns of growth and configurations of dopamine on the anatase (101) TiO2 surface, with reference to the archetype of 1,2-dihydroxybenzene ligands, i.e. cathecol.[3] At low coverage, the isolated dopamine molecule prefers to bend towards the surface, coordinating the NH2 group to a Ti5c ion. Increasing the dopamine coverage, we observed unexpected effects and proton transfers that largely stabilize the self-assembled monolayer.

References

[1] T. Paunesku et al. Nat. Mater. 2003, 2, 343*346.

[2] T. Rajh et al. Nano Lett. 2004, 4, 1017*1023.

[3] L. Liu et al. J. Am. Chem. Soc. 2011, 133, 7816*7823.

O 61.10 Wed 17:15 H25

Reaction Pathways in Heterogeneous Photoreforming of Tertiary Alcohols — •Moritz Eder, Carla Courtois, Kordula Schnabl, Constantin A. Walenta, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstraße 4, 85748 Garching, Germany

Tertiary alcohols are an ideal model system to investigate mechanisms in photocatalysis. Being organic hydroxyl carriers, they are suitable precursor materials for waste-water purification and biomass conversion. In this talk, we present our most recent results on platinum-loaded titania(110). It is shown that semiconductor photocatalysis selectively enables new reaction pathways, which are not accessible by thermal or conventional chemical methods.

O 62: Poster Wednesday: Topology and Symmetry-Protected Materials

Time: Wednesday 17:45–20:00 Location: Poster B1

O 62.1 Wed 17:45 Poster B1

Probing topological superconductivity in Indium doped topological crystalline insulator using high resolution photoemission spectroscopy — •Sangeeta Thakur[1,2,4], Deepnarayan Biswas[1], Akansha Singh[3], Pransjit Sen[3], K. Srinivas[1], A. Thamizhavel[1], Giovanni Di Santo[2], L. Petaccia[2], and K. Maiti[1] — [1]Tata Institute of Fundamental Research Colaba Mumbai India — [2]Elettra Sincrotrone Trieste, Trieste, Italy — [3]Harsh-Chandra Research Institute, HBNI, Allahabad, India — [4]Freie Universität Berlin, Institut für Experimentalphysik, Berlin, Germany

Pb0.6Sn0.36In0.04Te single crystals were investigated by high resolution photoemission spectroscopy to probe the topological superconductivity predicted for indium doped topological crystalline insulator (TCI). XRD measurements on Pb0.6Sn0.36In0.04Te confirm the rocksalt structure peculiar for TCI. Angle resolved photoemission spectra show the signature of Dirac cone surface states which gives evidence for an inverted band structure as in the pristine Pb0.6Sn0.36Te TCI sample. The experimental valence band spectra can be explained reasonably well by the theoretical calculations. Presence of topological surface state makes Pb0.6Sn0.36In0.04Te a potential material to find the topological superconductivity in TCI.

O 62.2 Wed 17:45 Poster B1

Study of ARPES, Magnetic and magneto-transport properties of Dy doped Bi2Te3 Topological Insulator — •Vinod Kumar Gangwar[1], Shiv Kumar[2], Yufeng Zhang[3], Prashant Shahi[4], Swapnil Patil[1], Eike Fabian Schwier[2], Kenya Shimada[2], Yoshiya Uwatoko[3], and Sandip Chatterjee[1] — [1]Department of Physics, Indian Institute of Technology (BHU) Varanasi 221005 — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima City, 739-0046 Japan — [3]Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan — [4]Department of Physics, D.D.U. Gorakhpur University, Gorakhpur 273009

Topological insulators are characterized by a gapped bulk state and gapless surface or edge states that is protected by time-reversal symmetry (TRS). TRS can be broken by magnetic impurities. To investigate the correlation between topological state and magnetism it is important to introduce magnetic elements into Topological insulators. In this study, we have synthesized the single crystals of Bi2-xDyxTe3 (x =0.06, 0.10, 0.16) and reported the effects of Dysprosium substitution on the topological properties in Bi2-xDyxTe3. XRD data indicate very good single crystallinity of Bi2-xDyxTe3 without any sign of secondary phase. We have measured the magnetization M(H) at different temperature and found that at low temperature it shows weak ferromagnetic ordering. From the ARPES and thermoelectric studies we found n-type nature of Dy doped Bi2Te3.

O 62.3 Wed 17:45 Poster B1

Theoretical study of the candidate material for type-II Weyl semimetal MoTe$_2$ using relativistic KKR method — •Ryota Ono[1], Yoshitaka Nakata[1], Alberto Marmodoro[2], Jan Minár[3], Hubert Ebert[2], Kazuyuki Sakamoto[4], and Peter Krüger[4] — [1]Department of Materials Science (Frontier Science Program), Graduate School of Science and Engineering, Chiba University, Chiba 263-8522, Japan — [2]Department of Chemistry, University of Munich, Butenandstr. 5-13, D-81377 München, Germany — [3]University of West Bohemia, New Technologies - Research Center, Univerzitni 8, 306 14 Plzeň, Czech Republic — [4]Graduate School of Science and Engineering and Molecular Chirality Research Center, Chiba University, Chiba 263-8522, Japan

Topological Weyl semimetals (TWS) are examples of Dirac materials, in which relativistic and quantum mechanical effects give rise to new physical features such as chiral anomaly in the transport of charged particles, giant anomalous Hall effect and emergence of Weyl fermions. TWSs can be classified into type-I and type-II according to whether they respect Lorenz invariance. MoTe$_2$ is a transition metal dichalcogenide (TMDC) and forms many phases, among which the T_d phase has been proposed as a candidate material for a type-II Weyl semimetal. Here we calculated the electronic structure of T_d MoTe$_2$ and explored its band structure around a Weyl point. Using the spin polarized relativistic KKR method, we also calculated ARPES in the one-step model which takes into account all matrix, surface and final state photoemission effects. The results are compared with experiment.

O 62.4 Wed 17:45 Poster B1

Type-II Weyl semimetals – spin-polarization, impurity scattering, and a polar instability — •Philipp Rüssmann[1], Phivos Mavropoulos[1,2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Department of Physics, National and Kapodistrian University of Athens, 15784 Zografou, Greece

Weyl semimetals are a new class of materials that host topologically protected crossings in their bulk electronic structure. Their intriguing transport properties have the potential to spark the development of radically new technologies based on topological semimetals. However, to fully realise their potential in the future, a microscopic understanding of the topological phase is required in terms of their nature of the phase transition and the functional response to impurities. In recent joint studies [1,2] we investigated the type-II Weyl semimetal candidates $MoTe_2$ and WTe_2 by combining DFT calculations with STM and ARPES experiments. Here, focusing on the theoretical side, we discuss evidence of a polar instability near the structural phase transition from the topologically trivial to the non-trivial Weyl phase in $MoTe_2$ [1]. In studying the response of both surface and bulk states to perturbations in topologically trivial WTe_2 and the stable Weyl phase in $MoTe_2$, we are able to uncover the existence of a universal response of surface- and bulk-derived topologically protected quasiparticles to naturally occurring defects in the crystals [2].

[1] A. P. Weber, *et al.* PRL **121**, 156401 (2018)
[2] P. Rüßmann, *et al.* PRB **97**, 075106 (2018)

O 62.5 Wed 17:45 Poster B1

Bulk band structure of Sb_2Te_3 — •Henriette Elisabeth Lund[1], Ann Julie Utne Holt[1], Martin Bremholm[2], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark — [2]Department of Chemistry and iNANO, Aarhus University, 8000 Aarhus C, Denmark

Sb_2Te_3 belongs to the class of materials known as topological insulators. The surface electronic structure of the material has been investigated with both angle-resolved photoemission spectroscopy (ARPES) and spin-resolved ARPES, but little is known about the bulk electronic structure of the material.

In the present study, the bulk and surface electronic structure of Sb_2Te_3 is investigated by means of ARPES performed at the ASTRID 2 synchrotron radiation facility in Aarhus, Denmark. The ARPES experiments reveal the presence of both two-dimensional and three-dimensional states in the band structure. The three-dimensional band structure is determined along high-symmetry directions in the Brillouin zone and compared to published band structure calculations.

O 62.6 Wed 17:45 Poster B1

Surface Berry curvature dipole in topological materials — •Dennis Wawrzik[1], Jhih-Shih You[1], Inti Sodemann[2], and Jeroen van den Brink[1,3] — [1]Institute for Theoretical Physics, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzerstr. 38, 01187 Dresden, Germany — [3]Department of Physics, Technical University Dresden, Helmholtzstr. 10, 01062 Dresden, Germany

Recently the research on understanding the effects of quantum geometry in novel materials has attracted considerable attentions both in theory and in experiment. A remarkable example is the Hall-like current that can occur in second-order response to an external electric field in materials with time-reversal symmetry but broken inversion symmetry, as a result of the dipole moment of the Berry curvature (BCD). However, the BCD is not allowed if a bulk has high crystalline symmetries. We show that for a proper chosen surface breaking some of these bulk symmetries one can find a non-vanishing surface BCD. The proposed effect could be observed in topological materials with a conducting surface like Weyl semimetals and TCIs.

O 62.7 Wed 17:45 Poster B1

Topological surface states in semi-metallic Tm monochalcogenides — •Chul-Hee Min[1], Chang Jong Kang[2], Katharina Kissner[1], Hendrik Bentmann[1], Dong-Choon Ryu[3], Woo Jae Choi[4], Yong-Seong Kwon[4], Volodymyr Zabolotnyy[1], Vladimir Hinkov[1], Byung-Il Min[3], and Friedrich Reinert[1] — [1]Universität Würzburg, EP7, Würzburg, Germany — [2]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08856, USA — [3]Department of Physics, PCTP, POSTECH, Pohang 37673, Korea — [4]Department of Emerging Materials Science, DGIST, Daegu 42988, Republic of Korea

Topological surface states with strongly localized 4f character have not been clearly identified in experiments yet. Analogous to hypothetically topological non-insulating rare earth materials, e.g. g-SmS and SmO [1,2], we propose Thulium monochalcogenides, $TmSe_{1-x}Te_x$, to be a very promising candidate to realize even topological Dirac or Weyl semimetals. The compounds having simple fcc structure show mixed valency overall, and insulating behaviors in resistivity. By means of ARPES, their Fermi surface maps and constant energy cuts will be present, which show a good agreement with our DFT calculation results. If the energy positions of 4f bands of Tm in DFT results can be renormalized with factor of 0.1, we can identify most of theoretical Fermi surface features, including the $4f$ surface states.

[1] D. Kasinathan, K. Koepernik, L. H. Tjeng, and M. Haverkort, Phys. Rev. B, 91 195127 (2015). [2] C.-J. Kang, H.-C. Choi, Kyoo Kim, and B. I. Min, Phys. Rev. Lett., 114, 166404 (2015).

O 62.8 Wed 17:45 Poster B1

Anomalous behavior of the electronic structure of $(Bi_{1-x}In_x)_2Se_3$ across the quantum-phase transition from topological to trivial insulator — •Friedrich Freyse[1], Irene Aguilera[2], Lada Yashina[3], Daria Tsukanova[3], Alexander Chaika[4], Carolien Callaert[5], Artem Abakumov[6], Joke Hadermann[5], Andrei Varykhalov[1], Emile Rienks[1], Gustav Bihlmayer[2], Stefan Blügel[2], Oliver Rader[1], and Jaime Sánchez-Barriga[1] — [1]Helmholtz-Zentrum Berlin — [2]Forschungszentrum Jülich and JARA — [3]Moscow State University — [4]Institute of Solid State Physics RAS — [5]University of Antwerp — [6]Skolkovo Institute of Science and Technology

Using spin- and angle-resolved photoemission and relativistic many-body calculations, we investigate the electronic structure of topological surface states (TSSs) across a topological quantum-phase transition in $(Bi_{1-x}In_x)_2Se_3$ bulk single crystals. By increasing x, we observe how a surface gap opens at the Dirac point of the initially gapless TSS of Bi_2Se_3, leading to the existence of massive fermions with non-zero spin polarization. The surface gap monotonically increases for a wide range of x values in both the topological and trivial sides of the phase transition. Our calculations reveal qualitative agreement with the experimental results all across the quantum-phase transition upon the systematic variation of the spin-orbit coupling strength. A non-time-reversal symmetry-breaking mechanism of bulk-mediated scattering processes that increase with decreasing spin-orbit coupling strength is proposed as explanation.

O 63: Poster Wednesday: Ultrafast Processes

Time: Wednesday 17:45–20:00 Location: Poster B1

O 63.1 Wed 17:45 Poster B1

Electron dynamics in MoS_2 after resonant optical excitation probed with different light polarizations — •Lasse Münster, Robert Wallauer, Johannes Reimann, Jens Güdde, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, 35032 Marburg

We will report on the application of time- and angle-resolved two photon photoemission (2PPE) with a high harmonic probe for the investigation of electron dynamics of MoS_2 in momentum space. For this purpose, we combined a high-repetition rate high-harmonic source with tunable femtosecond pump pulses and a 3D (k_x, k_y, E) electrostatic electron spectrometer [1].

We used this setup to study the electron dynamics in the conduction band of MoS_2 after resonant optical excitation at the $\overline{\text{K}}$-point with different polarizations of pump- and probe pulses. In addition to the excitation into the conduction band, we observe non-resonant 2PPE from the valence band which can be suppressed by using cross-polarized pump and probe pulses. Within our time-resolution of better than 50 fs, we observe an instantaneous occupation of the conduction band at $\overline{\text{K}}$ followed by an ultrafast transfer to the conduction band minimum at $\overline{\Sigma}$.

[1] R. Wallauer et al., Appl. Phys. Lett. 109, 162102(2016).

O 63.2 Wed 17:45 Poster B1

Quenching of charge density wave states in ultrafast transmission electron microscopy — •Till Domröse, Thomas Danz, and Claus Ropers — 4th Physical Institute - Solids and Nanostructures, University of Göttingen, Germany

Ultrafast transmission electron microscopy (UTEM) allows for investigation of nanoscale dynamics in a laser-pump/electron probe scheme [1]. Employing photoemission from a Schottky emitter, the Göttingen UTEM provides spatial resolution down to the subnanometer regime with down to 200fs temporal resolution [2].

Here, we present a time-resolved investigation of charge density wave (CDW) state quenching in UTEM. The diffraction pattern of 1T-TaS$_2$ in its nearly-commensurate (NC) phase gives insights into structural dynamics triggered upon optical excitation by analyzing diffraction intensities associated with the periodic lattice distortion (PLD) coupled to the CDW. The temporal evolution of the CDW amplitude and the transient lattice fluctuations are followed with femtosecond resolution over a range of excitation fluences. Following an initial quench of the CDW/PLD amplitude in the NC phase, we observe a partial recovery within few picoseconds and the excitation of a broad phonon population.

[1] A. H. Zewail, Science 328, 187 (2010)
[2] A. Feist et al., Ultramicroscopy 176, 63 (2017)

O 63.3 Wed 17:45 Poster B1

Energy-resolved measurement and simulation of hot electron transport in Au/Fe/MgO(001)

— •Jan Beckord[1], Yasin Beyazit[1], John Thomas[1], Ping Zhou[1], Detlef Diesing[2], Uwe Bovensiepen[1], and Manuel Ligges[1] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Faculty of Chemistry, University of Duisburg-Essen, 45141 Essen, Germany

We have established a new time-resolved, two-photon photoemission (tr-2PPE) technique, where the sample is pumped from the back side through a transparent substrate and subsequently probed from the front side. We apply this technique to Au/Fe/MgO(001) samples with various gold thicknesses and obtain energy-resolved transport velocities from the temporal shifts of the tr-2PPE signal. To understand the influence of the hot electron lifetimes in Au and Fe and other experimental parameters on these time shifts, we simulate the ballistic transport equation in this particular system both analytically and numerically. The simulation is then compared to our experimental results to extract the energy-dependent ballistic velocities. Our obtained values are consistent with previous, not energy-resolved measurements and comparable to theoretical values predicted from band-structure calculations. This study was funded by the DFG through SFB1242.

O 63.4 Wed 17:45 Poster B1

Ultrafast miniaturised pulsed electron gun for time-resolved LEED

— •Dennis Epp, Gero Storeck, Max Lukas Kroll, Murat Sivis, and Claus Ropers — IV. Physical Institute, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Solid state surface systems display complex structural and electronic phases, with properties that may drastically differ from the bulk [1]. The coupling between electronic, lattice and spin degrees of freedom can be studied by ultrafast techniques. The structural dynamics associated with transitions between different phases can be studied by the recently developed method of Ultrafast Low-Energy Electron Diffraction (ULEED) [2, 3]. In this method, a miniaturized laser-driven photoelectron source generates ultrashort low-energy electron pulses to probe pump-induced changes to the surface structure in a stroboscopic manner. In recent works, we employed millimetre- and a micrometre-sized photoelectron guns [2, 3]. The reduced outer diameter of both electron sources allows for a small working distance from the sample, minimizing dispersive electron pulse broadening and reducing shadowing on the detector in backscattering. Temporal resolutions down to 16 ps (millimetre-gun) and 1ps (micrometre-gun) are demonstrated. This contribution will describe the fabrication of the electron beam systems, measured beam properties and first applications. Further strategies to facilitate ULEED with sub-picosecond temporal resolution will be discussed. [1] J. M. Kosterlitz. & D. J. Thouless, J. Phys. C 6, 1181*1203 (1973). [2] G. Storeck et al., Structural Dynamics 4, 044024 (2017). [3] S. Vogelgesang, et al., Nature Physics 14,184-190 (2018).

O 63.5 Wed 17:45 Poster B1

Towards time resolved photoemission spectroscopy using a circularly polarized fs-XUV light source

— •Pascale Klaeger[1], Sebastian Emmerich[1], Jonas Hoefer[1], Sebastian Hedwig[1], Johannes Stöckl[1], Benito Arnoldi[1], Ofer Kfir[2], Claus Ropers[2], Benjamin Stadtmüller[1], and Martin Aeschlimann[1] — [1]University of Kaiserslautern and research center OPTIMAS, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Georg-August-Universität Göttingen, IV. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The combination of photoelectron spectroscopy with XUV- or soft x-ray radiation with circular polarization offers the intriguing opportunity to determine not only the band structure of solids but also to gain insight into the orbital character and the symmetry of the electronic states in these systems. Such radiation was so far mainly available at large scale facilities such as synchrotron light sources. Recent progress in high harmonic generation has demonstrated a novel way to create circularly polarized fs-XUV light on a laboratory scale[1,2]. Here, we show the implementation of the so called MAZEL-TOV device[2] into our HHG beamline and discuss our first ARPES data results obtained with circularly polarized fs-XUV radiation for ferromagnetic surfaces.

[1]O. Kfir et al., Nat. Phot. 9, 99 (2015) [2]O. Kfir et al., Appl. Phys. Lett. 108, 211106 (2016)

O 63.6 Wed 17:45 Poster B1

Oscillating kinetic energy in time-resolved photoemission

— •Xinwei Zheng[1], Kamil Bobowski[1], Dominic Lawrenz[1], Robert Carley[2], Beatrice Andres[1], Cephise Cacho[3], Richard Chapman[3], Emma Springate[3], Serguei Molodtsov[2], and Martin Weinelt[1] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimalle 14, 14195 Berlin, Germany — [2]European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Germany — [3]Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK

We measured ultrafast time-resolved photoemission spectra on Gd (0001) and W (110) with an IR pump, XUV probe set up at the Artemis laser facility. We observed an oscillating kinetic energy of the photoemitted electrons before time zero. Such oscillations have been observed on the surface state of Gd by Bovensiepen *et al.* [1]. They described the oscillations with a ponderomotive acceleration of the emitted photoelectrons in a transient grating formed by the interference between the incident and reflected parts of the pump pulse. We performed a further investigation on these oscillations by varying the wavelengths of the pump pulse and found that the amplitude and the phase of the oscillations are pump wavelength-dependent. They show different behavior than predicted by the ponderomotive acceleration model. By comparing the amplitude of the oscillations on different bands, we discovered that the oscillating kinetic energy depends on the initial state of photoemission.

[1] Bovensiepen *et al.*, Phys. Rev. B, **79**, 045415 (2009)

O 63.7 Wed 17:45 Poster B1

Surface motion of femtosecond-laser excited silicon films

— Tobias Zier[1], •Marie Kempkes[1], Sabrina Schuster[1], Lukas Nöding[1], J. Gaudin[2], P. Martinez[2], V. Blanchet[2], D. Descamps[2], S. Petit[2], A. Lévy[3], and Martin E. Garcia[1] — [1]Theoretische Physik, Universität Kassel, Kassel, Germany — [2]CEntre Lasers Intenses et Applications, Talence, France — [3]Institut des Nanosciences de Paris, France

Surfaces are active regions that exhibit various effects, like, structural reconstructions, already in the thermodynamic ground state. The underlying reason for most of these effects is the broken symmetry at the surface, which modifies the interatomic bonding of surface atoms. After an intense femtosecond-laser pulse the interatomic bonding characteristic of the whole irradiated area is changed due to the induced non-equilibrium conditions, which are characterized by an extremely hot electronic system and nearly unaffected room temperature atoms. Therefore, the bonding of surface atoms is modified twice after a femtosecond-laser excitation, which makes a prediction for the surface behavior non-trivial. We examined the surface response to a femtosecond-laser irradiation by performing ab initio MD simulations of a thin silicon film using our code CHIVES (Code for Highly excIted Valence Electron Systems). Our results can directly be compared to recent time-resolved optical measurements, thus allowing us to unravel the surface response to femtosecond-laser excitation on an atomistic level.

O 63.8 Wed 17:45 Poster B1

Electron-Phonon coupling in non-equilibrium: tr-RHEED on few monolayer Pb/Si(111) films

— •Tobias Witte, Bernd Hafke, Christian Brand, and Michael Horn-von Hoegen — Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

The recent advances in temporal resolution of electron diffraction experiments raised a multitude of questions regarding non-equilibrium dynamics of optically excited systems. Here, the response of the phonon system of few monolayer (ML) thin Pb/Si(111) films upon fs-IR laser excitation is investigated. This system is known for exhibiting different quantum well states for even or odd layers which should influence the electron phonon interaction. Employing time-resolved reflection high-energy electron diffraction the mean squared displacement of the surface atoms is analyzed for different Pb film thicknesses

θ_{Pb}. The excitation time constant is found to be almost independent of the layer thickness for coverages of 3 ML $\leq \theta_{\mathrm{Pb}} \leq$ 15 ML. The average value of $\tau_{\mathrm{exc}} = 3.2 \pm 0.4$ ps is significantly slower than expected from a two temperature model ($\tau_{\mathrm{TTM}} <$ 1 ps). This discrepency is discussed with respect to the non-thermal lattice model[1].

[1] L. Waldecker et al. - Phys. Rev. X 6, 021003 (2016)

O 64: Poster Wednesday: Plasmonics and Nanooptics

Time: Wednesday 17:45–20:00 Location: Poster B1

O 64.1 Wed 17:45 Poster B1

Photoemission electron microscopy using a 200 kHz high-order harmonic source — •Jan Vogelsang, Lukas Wittenbecher, Sara Mikaelsson, Chen Guo, Cord L Arnold, Anne L'Huillier, and Anders Mikkelsen — Department of Physics, Lund University, 221 00 Lund, Sweden

Ultrafast photoemission electron microscopy (PEEM) combines the high temporal resolution of short laser pulses with the high spatial resolution of electron microscopy. It elegantly circumvents the well-known problem of electron pulse dispersion by photoemitting and imaging electrons directly from a sample.

We developed an OPCPA laser system at 200 kHz repetition rate that drives the generation of high-order harmonics in an Ar gas jet. In combination with a spectral phase and amplitude pulse shaper, this system becomes a versatile tool to perform ultrafast PEEM experiments at a wide range of laser pulse energies and frequencies from the IR to the XUV.

We introduce the upgrade of the laser system driving high-order harmonic generation with a pulse energy of 10 to 15 uJ in the few-cycle regime. Additionally, first results of ultrafast PEEM experiments on both plasmonic and semiconductor nanostructures with varying dimensionality are shown.

O 64.2 Wed 17:45 Poster B1

Symmetry-induced coupling of plasmonic metasurfaces and $\mathbf{WS_2}$ — •Florian Spreyer[1], Feng Shun[2], Yu Ting[2], and Thomas Zentgraf[1] — [1]Department of Physics, University of Paderborn, Warburger Straße 100, 33098 Paderborn, Germany — [2]Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore

Recent studies show great potential for transition metal dicholgenides (TMD) and their optical application. By downscaling TMD*s to a monolayer flake of atomical thickness, TMD*s become semiconductors with a direct band gap. These monolayer flakes can be used to fabricate hybrid metasurfaces combining plasmonic nanoantennas and a monolayer of TMD. Hybrid metasurfaces with TMD*s with a band gap in the visible regime show great potential for an enhanced light matter interaction for nonlinear applications. Here we, investigate the coupling between a metasurface made of plasmonic C3 gold nanoantennas and a monolayer of tungsten disulfide (WS_2). We present recent results of the characterization of WS_2 flakes transferred to different substrates. By using photoluminescence and nonlinear measurements, we locate monolayers of WS_2 and the orientation of the symmetry axis. On top of the WS_2, we fabricate the plasmonic nanoantennas with different orientations and study their influence on the nonlinear properties by SHG spectroscopy.

O 64.3 Wed 17:45 Poster B1

Electron-induced photon injection at single-mode glass fibres in transmission electron microscopy — •Vincent Hock, Christopher Rathje, Niklas Müller, Holger Koch, and Sascha Schäfer — University Oldenburg

Transmission electron microscopy (TEM) provides a versatile platform for the investigation of electron-light interaction at the nanoscale [1]. Utilizing femtosecond electron pulses and transient localized light fields, ultrafast TEM experiments have opened new avenues for the coherent optical control of free-electron wave packets [2-4]. Translating these developments to an optical control of continuous electron beams remains challenging. Here, we report on the current status of our investigations on high-energy electron beams interacting with guided modes in optical fibres. Utilizing a home-build TEM sample holder incorporating an on-axis tapered glass fibre, we demonstrate electron-induced light injection into the single-mode fibre with a spatially inhomogeneous injection efficiency. Photon count rates, light spectra and photon statistics are discussed considering different electron-light coupling mechanisms, including coherent transition radiation as well as cathodoluminescence processes.

[1] García de Abajo, Rev. Mod. Phys. 82, (2009)
[2] Barwick, Flannigan, Zewail, Nature 462, 902-906 (2009)
[3] Feist et al. Nature 521, 200-203 (2015)
[4] Priebe, Rathje et al., Nat. Photonics 11, 793-797 (2017)

O 64.4 Wed 17:45 Poster B1

Quantification of the chemical enhancement contribution to surface enhanced Raman scattering (SERS) — •Bonito Thielert[1,2], Bo Liu[1,2], Rainer Stosch[3], and Peter Lemmens[1,2] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]Abt. 3.1, PTB, Braunschweig, Germany

In our aim to quantify chemical enhancement (CM) in SERS we study light-matter interactions of molecules on dedicated Au nanorod arrays. The latter are based on AAO substrates and allow tunable geometries and interaction parameters of the plasmonic array. Using Rhodamine 6G and Malachite Green we analyze the effect of light-induced degradation and mobility on the SERS intensity. Work supported by DFG-RTG 1952/2 "NanoMet" and Braunschweig-IGSM.

O 64.5 Wed 17:45 Poster B1

Excitation Pathways in Nonlinear Photoemission visualized through Photon-Plasmon Spin-Orbit Mixing — •Michael Hartelt[1], Grisha Spektor[2], Eva Prinz[1,3], Anna-Katharina Mahro[1], Deirdre Kilbane[1,4], Meir Orenstein[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Department of Electrical Engineering, Technion - Israel Institute of Technology, Haifa, Israel — [3]Graduate School for Excellence Materials Science in Mainz, Germany — [4]Telecommunications Software & Systems Group, Waterford Institute of Technology, Waterford, Ireland

Light carries spin angular momentum (SAM) in the form of its helicity, but it can also carry orbital angular momentum (OAM) in the form of vortex beams. This phenomenon was also shown for surface plasmon polaritons (SPP), where a phase vortex can be generated in 2D. We measured the interaction between light carrying axial SAM and plasmon vortices with high order transverse OAM.

The interaction is mediated via two-photon absorption on a gold surface, imprinting the resulting angular momentum mixing into matter by excitation of electrons that are photo-emitted into vacuum and detected by PEEM. We show that this interaction leads to both single and double photon-plasmon angular momentum mixing processes. The different mixing processes can be identified with specific quantum pathways of the electron excitation. In an interferometric pump-probe experiment, we isolate these pathways by frequency decomposition of the phase-resolved signal.

O 64.6 Wed 17:45 Poster B1

A compact optical-pump/THz-probe spectrometer based on sub-diffraction field confinement — •Michael Seidel and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

Optical-pump/THz-probe spectroscopy presents a powerful scheme for contact-free detection of transient carrier mobilities and relaxation dynamics. In this contribution, we present a novel experimental approach to realize time-resolved time-domain THz spectroscopy (tr-THz-TDS) based on a compact mode-locked fiber laser, efficient frequency conversion and photoconductive detection. Specifically, this approach employs sub-diffraction confinement and optical mode-matching in order to enhance sample excitation and signal strength. The instrument is used to characterize transient carrier dynamics in organic electronic materials and devices.

O 64.7 Wed 17:45 Poster B1

Phase-resolved detection of strong terahertz nearfields —

•Moritz Heindl and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

Table-top schemes to generate ultrafast radiation in the terahertz spectral range enable access to strong sub-picosecond field transients at increasingly high repetition rates. This opens up novel schemes for ultrafast probing and control of quantum systems. Nanostructures, e.g., micro-antennas and micro-slits, can further enhance the electric fields by orders of magnitude. The exact knowledge of the absolute local field strengths is highly desirable and has been realized with electron nearfield streaking [1], electron microscopy [2] and electro-optical sampling [3]. Here, we present an all-optical widefield approach to detect the absolute values of the THz electric fields on a subwavelength scale. This provides a defined platform to study THz field-driven dynamics in complex nanostructures.

[1] L. Wimmer et al., "Terahertz control of nanotip photoemission", Nature Physics 10, 432 (2014)
[2] A. Ryabov et al., "Electron microscopy of electromagnetic waveforms", Science 353, 374 (2016)
[3] F. Blanchard et al., "Improving time and space resolution in electro-optic sampling for near-field terahertz imaging", Opt. Lett. 41, 4645 (2016)

O 64.8 Wed 17:45 Poster B1

Influence of cesium adsorption on plasmoemission from gold surfaces — •Jan-Henrik Herrig[1,2], David Janoschka[1,2], Pascal Dreher[1,2], Michael Horn-von Hoegen[1,2], and Frank-J. Meyer zu Heringdorf[1,2] — [1]Faculty of Physics & CENIDE, Lotharstraße 1, 47048 Duisburg — [2]University of Duisburg-Essen, Duisburg, Germany

It is known that the superposition of a SPP-field and an incident light field leads to the non-linear emission of electrons. Recently, a photoemission electron microscopy (PEEM) experiment was used to show that the pump-probe contribution to the electron yield originates from the SPP's longitudinal component. Plasmoemisson, in which electrons are liberated from the metal surface by the SPP's electrical field alone, however, is dominated by the SPP's transverse component. To enable a second order emission process, the high work function of the used Au-surfaces is routinely decreased by the adsorption of sub-monolayer coverages of cesium. Until now, it was not known whether cesium adsorption changes which one of the field components dominates the plasmoemission yield. By careful analysis of the spatial modulation of the electron yield as function of cesium coverage in a plasmonic standing-wave experiment we can spatiotemporally separate the emission from different field components. Here we use light- and SPP-pulses to investigate whether there is a change in the spatial distribution of the electron yield induced by the cesium adsorption. We show evidence that sub-monolayer coverages of cesium do not have substantial influence on the character of the emission processes.

O 64.9 Wed 17:45 Poster B1

Ultrafast time-resolved photoemission electron microscopy of indium arsenide nanowires with variable crystal phase — •Lukas Wittenbecher[1,2], Jan Vogelsang[1], Sebastian Lehmann[1], Kimberly Dick Thelander[1], Donatas Zigmantas[2], and Anders Mikkelsen[1] — [1]Department of Physics, Lund University, Sweden — [2]Chemical Physics, Lund University, Sweden

The III-V nanowire (NW) technology platform has reached a level of advancement that allows atomic scale control as well as flexible device integration. In particular, controlled axial stacking of segments with Wurtzite (Wz) and Zinc blende (Zb) crystal phase is uniquely possible in the NWs. We have previously found that multiphoton electron excitations from indium arsenide (InAs) NWs with Wz and Zb segments can controllably varied across the crystal segments that also retain their electronic properties to the smallest possible scales. However, the effect of the crystal phase on the ultrafast dynamical behavior of photo-excited electrons in these NWs has so far not been explored.

In the present study we combine photoemission electron microscopy with ultrafast optical pump-probe techniques to investigate the photoexcitation dynamics in InAs NWs with alternating Wz and Zb segments with 50 nm spatial and 20 fs temporal resolution. We focus on the initial stages of the electron relaxation process, and we interpret the observed signals as signatures of the thermalization and cooling of photo-excited electrons. We find small differences in the observed dynamics between Wz and Zb segments phase depending on the excitation conditions.

O 64.10 Wed 17:45 Poster B1

Revealing the magneto-plasmonic enhancement in Bi:YIG/Au hybrid nanostructures — Spyridon Pappas and •Evangelos Papaioannou — Department of Physics, TU Kaiserslautern

Magnetoplasmonics allows to explore the influence of the strong localization of light, enabled by resonant plasmonic structures, on the response of magneto-optically active adjacent materials. In this work, we demonstrate experimentally the anomalous enhancement of the longitudinal magneto-optic Kerr effect of bismuth substituted yttrium iron garnet films, induced by localized surface plasmons in embedded gold nanoparticles. Additionally, we reveal the underlying mesoscopic nanoscopic near-field mechanism. In order to gain insight into the exact origin of the anomalous magneto-optic response of the hybrid metastructure, we performed far-field simulations, as well as near-field analysis. The far-field simulations reproduce very well the features of the magneto-optic response in the spectral vicinity of the relevant plasmonic resonances. The near-field studies reveal an enhancement of the purely magneto-optically induced field at a spectral position, which correlates with the lateral dimensions of the nanoparticles, and is different from the spectral position of the main plasmon resonance. The exact correlation of the origin of the plasmon-induced effects on the properties of the adjacent magneto-optic materials, as well as the near-field mapping of the enhanced polarization conversion efficiency, can have a high impact on the engineering of hybrid magneto-plasmonic metastructures.

O 65: Poster Wednesday: Surface Structure, Epitaxy and Growth

Time: Wednesday 17:45–20:00 Location: Poster B1

O 65.1 Wed 17:45 Poster B1

Polymorphic expressions of ultrathin oxidic layers of Mo on Au(111) — Taehun Lee[1], Yun-Jae Lee[1], Krisztián Palotás[2], Catherine Stampfl[3], and •Aloysius Soon[1] — [1]Department of Materials Science & Engineering, Yonsei University, Seoul 03722, Korea — [2]Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary — [3]School of Physics, The University of Sydney, NSW, 2006, Australia

Ultrathin oxidic layers of Mo (O/Mo) on the Au(111) support have been investigated using first-principles density-functional theory calculations. Various polymorphic structural models of these O/Mo layers are proposed and compared with previous experimental results – covering both spectroscopic and microscopic approaches of characterization. We find that, through the control of metal-oxygen coordination in these ultrathin oxidic O/Mo films on Au(111), the oxidation state of Mo atoms in the O/Mo layers can be modulated and reduced without intentional creation of oxygen vacancies. This is also assisted by a charge transfer mechanism from the Au substrate to these oxidic films, providing a direct means to tune the surface electronic properties of ultrathin oxide films on metal substrates.

O 65.2 Wed 17:45 Poster B1

Structural investigation of strain induced effects in a Dy-Ag surface alloy — •Sina Mousavion[1], Johannes Seidel[1], Lu Lyu[1], Maniraj Mahalingam[1], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany

Studies of intermetallic compounds using lanthanide metals on noble metals have been subject of numerous studies due to their tunable structure as well as their electronic and magnetic properties [1]. In this study we focus on the structural properties of a Dysprosium-Ag surface alloy formed on the Ag(111) surface. Using LEED and STM, we observe the formation of a short range ordered Dy-Ag structure with an additional Moiré-like pattern. This is in contrast to most surface alloys which usually form a uniform Sqrt(3)xSqrt(3) structure on Ag(111). This intriguing surface structure can be explained by a non-uniform lattice strain in the adsorbate system due to the size mismatch of Dy and Ag. We propose that the formation of a Moiré pattern of the surface alloy can be used to control the structure formation of adsorbates on this surface alloy. [1] e.g., Nano Lett., 16, 4230-4235 (2016)

O 65.3 Wed 17:45 Poster B1

Two-dimensional CuI on Cu(111): A first-principles investigation — •Giyeok Lee, Taehun Lee, and Aloysius Soon — Department of Materials Science & Engineering, Yonsei University, Seoul 03722, Korea

Of late, copper iodide (CuI), a *p*-type transparent semiconductor at room temperature, has been proposed as a choice material for various potential applications – from a hole conductor to a bipolar diode, forming a two-dimensional heterojunction with various *n*-type materials. However, the controlling the atomic structure of ultrathin (or interfacial) CuI layers for these targeted applications is challenging due to the existence of various polymorphic expressions (γ – zincblende structure as thermodynamic product, β – hexagonal phase, and α – rocksalt structure). The structures of ultrathin layers are determined by the orientation of metal substrates (e.g. Cu(100) and Cu(111)) and the surface coverage of precursors (e.g. $I_{2\,(g)}$ or $KI_{\,(aq)}$) used. In this work, we have performed van der Waals-corrected density-functional theory calculations to examine the initial/early stages of CuI ultrathin film formation on Cu(111) within the framework of *ab initio* atomistic thermodynamics, and report detailed surface atomic structures with their associated surface thermodynamics and electronic structure properties.

O 65.4 Wed 17:45 Poster B1

In-situ analysis of ultra-thin alkali metal films using optical transmission spectroscopy — •Hendrik Mathies Wrigge, Thomas Dziuba, Joerg Malindretos, Angela Rizzi, and Martin Wenderoth — IV. Physikalisches Institut, Georg August Universität Göttingen, Germany

Controlling the thickness of ultra-thin alkali metal films is a challenging task. Standard calibration techniques using e.g. ambient AFM, fail due to the high chemical reactivity of these metals. In this contribution, we present an alternative approach based on an in-situ optical transmission spectroscopy. Films are prepared by depositing pure alkalimetal from a dispenser on a glass substrate under UHV condition. While deposition, the optical transmission of the film is measured over a broad spectral range from 300 nm up to 1000 nm continuously (30 second per spectrum). We analyze distinct spectral features, which change according to the film thickness. Applying the scattering theory of non-spherical particle [1,2], the spectral features can be assigned to the film thickness and its nanoscopic structure. For comparison, we measured thin Ag films in the same setup. For Ag films, thickness as well as the structure is analyzed using AFM. In summary, our optical setup is able to measure deposition rate down to submonolayers per minute.

Work supported by DFG through SPP 1666

Reference: [1] K. Lance Kelly *et al.*, J.Phys. Chem. B, 107, 668-677 (2003) [2] Luis J. Mendoza Herrera *et al.*, Journal of Applied Physics 116, 233105 (2014)

O 65.5 Wed 17:45 Poster B1

Verkleinerung der mechanischen Spannungen im System <Aluminium-Anodenoxid des Aluminiums> — Basov Georgi und •Vladimir Schulgov — Belorussische Staatliche Universität für Informatik und Radioelektronik(BSUIR) Brovka Str. 6 BY 220013 Minsk Belarus

Das Aluminium und seinen Anodenoxid stellen die mehrschichige Struktur mit verschiedenen Eigenschaften von den Materialien vor. Im Laufe der Herstellung und der Betrieb können in ihr die thermischen Spannungen entstehen, die zur Übertretung der Ganzheit von Isolationsdeckung führen.

Im Laufe des Wachstums an der Trennungsgrenze Al - Al2O3 entsteht die Zone der plastischen Deformation des Aluminiums, in der die Relaxation des Teiles von der elastischen Spannungen geschieht. Sie ist ungefähr drei Radien des Zellegrunds vom porösen Oxids gleich. Der Zelledurchmesser des porösen Oxids nimmt proportional zur Anodisierungsspannung zu. Deshalb muss man die poröse Anodisierung bei den grossen Grössen der Anodisierungspannung durchführen.

Die vergleichende Einschätzung des Niveaus der thermischen Spannungen in den Filmen führten nach der Messung der Probedurchbiegung durch, der in die inneren Spannungen im Temperaturbereich 298 - 623K nachgerechnet wurde.

Schlussfolgerungen: Die Zusätze der Oberflächenaktivstoffen lassen mehr als in 2 Male die Größe der Durchbiegung und in 10 Male das Niveau der Spannungen zu verringern, die bei den Hochtemperaturbehandlungen an der Trennungsgrenze Al - Al2O3 entstehen sind.

O 65.6 Wed 17:45 Poster B1

Growth studies of Fe_3O_4 on $SrTiO_3$(001) by SPA-LEED — •Andreas Alexander, Jascha Bahlmann, and Joachim Wollschläger — Universität Osnabrück Fachbereich Physik, Barbarastr. 7, 49076 Osnabrück

Because of its electric and magnetic properties, Fe_3O_4 (Magnetite) is a promising candidate for spintronic applications, such as magnetic tunneling junctions (MTJs) or magnetic data storage (Magnetoresistive Random Access Memory = MRAM). Previously, magnetite films were grown on lattice matched MgO substrates. Here, we study Fe_3O_4 epitaxy on $SrTiO_3$(001) (lattice mismatch -7.5%) by means of high resolution low energy electron diffraction with spot profile analysis (SPA-LEED) to shed light on strain effects. The magnetite films were grown by stepwise deposition and linescans were performed after each deposition step for different energies.

Due to the lattice mismatch an (111) oriented epitaxial interface layer is observed first. The thickness depends on growth conditions. Thereafter, the magnetite film reorientates and grows with (001) direction. Additionally, the profile analysis of the diffraction spots reveals information about the surface morphology, such as atomic steps, roughness or surface defects.

O 65.7 Wed 17:45 Poster B1

Strain induced enhanced magnetization of ultrathin epitaxial $NiFe_2O_4$ films on $SrTiO_3$(001) — •Jari Rodewald, Tabea Nordmann, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Ultrathin epitaxial ferrite films as $NiFe_2O_4$ are in the focus of spintronics owing to their semiconducting and ferrimagnetic properties. Thus, they are well-suited to be used as spin filters due to spin dependent tunneling barrier. Here, the homogeneity of the films is essential to form tunneling barriers. Furthermore, the cation ordering on the different sublattices of the inverse spinel structure determines the magnetic properties of the ferrite films which is crucial for the performance as a spin filter. Therefore, the formation of ferrite films has to be carefully controlled if high quality devices are aimed for.

Hence, in this work ultrathin $NiFe_2O_4$ films of different thicknesses are prepared via reactive molecular beam epitaxy (RMBE) on $SrTiO_3$(001). Chemical composition and structural ordering at the surface are examined by x-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED), respectively. In order to investigate structural strain and ordering effects in the films, synchrotron radiation based grazing incidence x-ray diffraction (SR-GIXRD) experiments are performed. Magnetic properties are characterized via superconducting quantum interference device (SQUID) magnetometry, revealing unexpectedly high magnetic moments exceeding bulk values of up to four times for ultrathin films below 13 nm film thickness.

O 65.8 Wed 17:45 Poster B1

Formation of cobalt ferrite by interdiffusion of CoO/Fe_3O_4 bilayers — •Jannis Thien, Jascha Bahlmann, Andreas Alexander, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

With their magnetic and electronic properties thin $CoFe_2O_4$ (CFO) films are among the most promising candidates for the development of spin filters at room temperature, where spin-polarized electron currents are generated due to the spin-dependent tunnelling barrier. Since the efficiency of spin-filtering greatly depends on the band structure of the material and the presence of defects, the fabrication of these films has to be carefully controlled if efficient spin filters are aimed for. To prepare thin CFO films pulsed laser deposition or sputter deposition is commonly used. Another approach of preparing CFO films might be the interdiffusion of CoO/Fe_3O_4 bilayers mediated by post-deposition annealing as recently shown for $NiFe_2O_4$ using Fe_3O_4/NiO bilayers.

Therefore, CoO/Fe_3O_4 bilayers were consecutively grown by reactive molecular beam epitaxy on $SrTiO_3$(001) and post-annealed at different temperatures afterwards. The film structure and chemical properties of the annealed bilayer system have been studied after each annealing step using synchrotron radiation by means of (grazing incidence)

X-ray diffraction and soft/hard X-ray photoelectron spectroscopy, respectively.

The measurements revealed interdiffusion of CoO and Fe_3O_4 films after an annealing temperature of 673K and probable formation of $Co_xFe_{3-x}O_4$.

O 65.9 Wed 17:45 Poster B1

N_2 physisorption on the KCl(100) surface — •Jochen Vogt — Chemisches Institut der Uni Magdeburg, Magdeburg, Germany

Molecular nitrogen is known to only weakly interact with ionic materials like NaCl and KCl [1,2]. Experimental information on the adsorbate structures is sparse so far [1]. This contribution compares results from quantitative low-energy electron diffraction (LEED) experiments for these systems. While in the case of N_2/NaCl(100) a p(1×1) symmetry is observed even at the lowest accessible temperature of 20 K, lattice mismatch induced strain causes a different behavior in the N_2/KCl(100) system. Here, the p(1×1) phase transforms into an oblique 2D phase of higher density at elevated N_2 partial pressure and temperatures below 40 K. For the p(1×1) phase, LEED I(V) analysis supports an adsorption site of N_2 on top of Na^+ on the NaCl substrate [1], while on the KCl(100) surface the N_2 molecules appear laterally displaced on the line connecting neighboring cations. This is interpreted in terms of strain-induced structural disorder that causes local coalescence of neighboring molecules. [1] J. Vogt, J. Chem. Phys. **137** (2012), 174705 [2] J. Vogt, H. Weiss, Z. Phys. Chem. **218** (2004), 973

O 65.10 Wed 17:45 Poster B1

From Fe_3O_4/NiO bilayers to $NiFe_2O_4$-like thin films through Ni interdiffusion — •Olga Kuschel[1], Ralph Buss[1], Timo Kuschel[2], Karsten Kuepper[1], and Joachim Wollschläger[1] — [1]Osnabrück University, Germany — [2]Bielefeld University, Germany

Ferrites with (inverse) spinel structure display a large variety of electronic and magnetic properties, making some of them interesting for potential applications in spintronics. Especially, $NiFe_2O_4$ thin films are of huge interest since they are magnetic insulators or semiconductors with spin dependent band gap. Therefore, they can be used as spin filters or for thermal induction of spin currents via the spin Seebeck effect. Furthermore, electrical charge transport and spin currents can be manipulated by the spin Hall magnetoresistance using $NiFe_2O_4$ thin films adjacent to nonmagnetic spin-Hall material.

For this purpose, thermally induced formation of nickel ferrite starting with a distinct Fe_3O_4/NiO bilayer grown on Nb-doped $SrTiO_3$(001) was investigated. After synthesis a systematic three-step annealing cycle was performed. After each annealing step surface crystallographic and 'bulk' electronic structure changes were investigated by means of low energy electron diffraction (LEED), soft and hard x-ray photoelectron spectroscopy (HAXPES). Furthermore, structural analysis before and after the overall annealing cycle were carried out employing x-ray reflectivity (XRR) and synchrotron-radiation-based x-ray diffraction (SRXRD), as well as element- and site-specific x-ray magnetic circular dichroism (XMCD) to analyze the resulting magnetic properties.

[1] O. Kuschel et al., Phys. Rev. B 94, 094423, (2016)

O 65.11 Wed 17:45 Poster B1

Structures and energetics of surface steps of SiC — •Kaori Seino[1,2] and Atsushi Oshiyama[1] — [1]Institute of Materials and Systems for Sustainability, Nagoya University, Nagoya, Japan — [2]X-Ability Co., Ltd., Tokyo, Japan

Silicon carbide (SiC) is a material of considerable interest due to applications in power semiconductors. Stepped surfaces of SiC are important from the viewpoint not only of a crucial role in epitaxial growth but also of substrates for epitaxial graphene. There exist, however, only a small number of theoretical *ab initio* studies of surface steps of SiC [1].

Here we present density functional theory (DFT) calculations of structural properties and energetics for surface steps of 3C-SiC(111) surfaces. The calculations are performed using the real-space DFT (RSDFT) program code [2]. In the present work, we reveal atom-scale structures of single-bilayer steps inclined toward different directions. Further, we discuss the energetics of the step structures by calculating step formation energies. Based on the results, the morphology of the surface steps during epitaxial growth could be discussed.

[1] K. Sawada, J.-I. Iwata, and A. Oshiyama, Appl. Phys. Lett. **104**, 051605 (2014).

[2] J.-I. Iwata, https://github.com/j-iwata/RSDFT.

O 65.12 Wed 17:45 Poster B1

SPA-LEED studies on the Sn/Ge(111) $(3 \times 3) \leftrightarrow (\sqrt{3} \times \sqrt{3})$ Mott-insulator to metal phase transition — •Fabian Thiemann, Semih Özdemir, Christian Brand, Bernd Hafke, Tobias Witte, and Michael Horn-von Hoegen — Universität Duisburg-Essen

An ordered adsorbate layer of 1/3 monolayer of Sn on a Ge(111) surface exhibits a reversible Mott-insulator to metal transition at 173 K [1, 2] which is accompanied by a structural transition from a (3×3) to $(\sqrt{3} \times \sqrt{3})$ superstructure. Employing spot-profile-analysis low-energy-electron-diffraction allowed the acquisition of high-resolution line profiles and thus an accurate determination of the temperature dependent intensity of the characteristic superstructure spots. Through temperature cycling of the sample starting from the (3×3) ground state at 110 K to the metallic $(\sqrt{3} \times \sqrt{3})$ phase at temperatures above the transition temperature of 173 K we followed the reversible phase transition through $k_{\parallel}$-dependent line profiles taken for each temperature step. The contribution to the spot intensity through the Debye-Waller factor and the structure factor were individually determined.

[1] J. Avila et. al., Phys. Rev. Lett. **82**, 442 (1999).

[2] A. V. Melechko et. al., Phys. Rev. B **61**, 2235 (2000).

O 65.13 Wed 17:45 Poster B1

2D Supramolecular Self-assembly of C8-BTBT on Cu(111) — •Sebastian Becker[1,3], Lu Lyu[1], Benjamin Stadtmüller[1,2], Sina Mousavion[1], Maniraj Mahalinam[1] und Martin Aeschliemann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [3]Department of Chemistry, University of Kaiserslautern, Erwin-Schrödinger-Straße 52, 67663 Kaiserslautern, Germany

Benzothieno[3,2-b]-benzothiophene (BTBT) is one of the most attractive core structures because of its chemical stability as well as its electronic properties and its derivatives with different end groups have been synthesized which demonstrate a very promising mobility up to 100 cm2V-1s-1. Here we use the VT-STM and LEED to systematically investigate the self-assemble behavior of monolayer 2,7 Dioctyl[1]-BTBT (C8-BTBT) on Cu(111). STM shows three different phases of C8-BTBT at 106 K. When increasing the sample temperature, phase transitions exist in different phases, which coincides with a temperature-dependent LEED measuring. Our findings will open insight into understanding of the mechanism of single-crystal organic semiconductor to further improve the performance.

O 65.14 Wed 17:45 Poster B1

Influence of the sample preparation on hydrogen-induced surface reconstruction on Pd(110) — •Robert Schindhelm[1], Markus Leisegang[1], Jens Kügel[1], and Matthias Bode[1,2] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Wilhelm Conrad Röntgen Center of Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg

The three main impurities to be considered when cleaning Pd(110) surfaces are hydrogen (H), carbon (C), and oxygen (O). Especially, H-induced vacancy rows reconstructions were investigated by STM [1,2]. We have systematically investigated the influence of some preparation parameters, i.e., the annealing temperature and the hydrogen pressure, on the temporal evolution of H-induced surface reconstructions by means of room-temperature STM. Whereas most results are in agreement with literature, our quantitative analysis regarding the relation between vacancy rows and adatom rows reveals some significant differences. We will discuss the suitability of these Pd(110) surfaces for studies of the direct [3] and remote [4] charge carrier-induced vibrationally excited motion of *cis*-2-Butene, a prominent example for molecular switches [3].

[1] E. Kampshoff *et al.* Surf. Sci. **360**, 55 (1996).

[2] M. Kralj *et al.* Surf. Sci. **600**, 4113 (2006).

[3] Kawai *et al.* Phys. Rev. Lett. **95**, 246102 (2005).

[4] Leisegang *et al.* Nano Lett. **18**, 2165 (2018).

O 65.15 Wed 17:45 Poster B1

Photoelectron holography – an experimentalist's approach to computer calculated reconstructions — •Matthias Gianfelice[1], Christopher Kohlmann[1,2], and Carsten Westphal[1,2] — [1]Experimental Pysics I - TU Dortmund University, Otto-Hahn-Str. 4a, D-44221 Dortmund — [2]DELTA - TU Dortmund University, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund

The determination of atom locations within surface structures is of great importance for basic science and for applications. Atomic force microscopy allows the analysis of the uppermost atomic layer, however this technique does not provide any information about the three-dimensional subsurface structure.

D. Gabor proposed a holographic approach suggesting electron waves for three-dimensional atom imaging. The electron wave length is in the order of the atom distances and thus should be well suited for the determination of atom structures. Unfortunately it is very hard to reconstruct atom images from a detection hologram because of non-isotropic electron scattering.

In this contribution we present recent progress on reconstructing three-dimensional atom images from electron holograms.

O 65.16 Wed 17:45 Poster B1

Thermal motion slows down the In/Si(111)(8x2)-(4x1) phase transition — •Marvin Krenz, Uwe Gerstmann, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn

The optically induced In/Si(111)(8x2)-(4x1) insulator-metal transition serves as a prototypical model for the interplay of electronic and structural degrees of freedom during photoreactions [1,2]. Interestingly, at 20 K, the photo-induced (8x2)-(4x1)phase transition occurs extremely fast, in the quantum limit, and requires only a few hundred femtoseconds [1]. Here we present ab initio molecular dynamics calculations on excited-state potential energy surfaces based on constrained DFT. The calculations that account for temperature effects at 100 K indicate that thermal motion has a small effect on the transition time with a tendency to a slightly slow down the transition.

[1] T Frigge et al., Nature 544, 207 (2017). [2] CW Nicholson et al., Science 362, 821 (2018).

O 66: Poster Wednesday: 2D Materials

Time: Wednesday 17:45–20:00 Location: Poster B2

O 66.1 Wed 17:45 Poster B2

Structure formation and electron dynamics of Pb intercalated graphene/metal interfaces — •Eva Sophia Walther[1], Christina Schott[1], Florian Haag[1,2], Dominik Jungkenn[1], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern — [2]Material Science in Mainz, JGU Mainz

Graphene is the most intriguing low dimensional material for future nano-electronics mainly due to its exceptional electronic properties with a Dirac cone-like spectrum and massless Dirac-Fermions. Yet, for electronic devices, it is necessary to find new ways to functionalize the electronic properties of graphene. One promising route to chemically manipulate graphene is the intercalation of heavy metal atoms between the graphene and the underlying substrate surface. This procedure cannot only suppress the interaction between the substrate surface and the graphene sheet but can also lead to the formation of a band gap at the Dirac-point [1]. Here, we present structural changes of the graphene/metal interfaces upon the adsorption and intercalation of Pb atoms using low energy electron diffraction and photoemission electron microscopy. Subsequently, we turn to the electron dynamics in this material system which was investigated by momentum-resolved photoemission spectroscopy. Our results allow us to correlate the electron dynamics to the vertical interactions of the graphene/metal interface prior to and after the adsorption Pb atoms. [1]I.I. Klimovskikh et al. ACS Nano 2017, 11, 368-376

O 66.2 Wed 17:45 Poster B2

A HR-XPS study of the formation of h-BN on Ni(111) from the two precursors, ammonia borane and borazine — •Philipp Bachmann, Fabian Düll, Florian Späth, Udo Bauer, Hans-Peter Steinrück, and Christian Papp — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen, Germany

Together with borazine, ammonia borane is a prominent precursor molecule for the formation of hexagonal boron nitride, which is of high interest as a 2D-material and graphene analog. Ammonia borane is also a possible solid hydrogen carrier with high storage density. Using X-ray photoelectron spectroscopy and temperature-programmed desorption, we investigated low-temperature adsorption and dehydrogenation during heating of borazine and ammonia borane on Ni(111) to form h-BN. For borazine, we observe the formation of disordered boron nitride above 300 K, which starts to form hexagonal boron nitride above 600 K. Ammonia borane shows multiple dehydrogenation steps at the boron and nitrogen atoms up to 300 K. This results in various BHxNHy species, including borazine-like intermediates, before the formation of disordered boron nitride and finally hexagonal boron nitride, analogous to the borazine decomposition. We acknowledge the SFB 953 "Synthetic Carbon Allotropes" for financial support.

O 66.3 Wed 17:45 Poster B2

Mechanical characterization of carbon nanomembranes and graphene via AFM nanoindentation and bulge testing — •Florian Paneff[1], Xianghui Zhang[1], Nikolaus Meyerbröker[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [2]CNM Technologies GmbH, 33609 Bielefeld, Germany

With the development of freestanding two-dimensional materials and nanomembranes, the precise characterization of the mechanical properties of these sheets has become an important challenge. It is thus beneficial to combine several methods to obtain more accurate results. Here we employed both bulge testing and nanoindentation performed in an atomic force microscope (AFM) to determine the elastic properties of these nanomembranes. In the former case a uniform pressure was applied to a membrane and the resultant deflection was recorded by the AFM, whereas in the latter case the AFM tip was positioned to the center of the same membrane and force-displacement curves were measured. Both pressure-deflection and force-displacement data were processed and compared with finite element method to determine the elastic properties of the membrane. In this contribution we will report the mechanical properties of carbon nanomembranes prepared from aromatic self-assembled monolayers via electron irradiation. Mechanical characterization of other nanomaterials, such as mono- and bi-layer CVD graphene, carbon nanosheets and pyrolized graphitic carbon, will also be discussed.

O 66.4 Wed 17:45 Poster B2

Structural and electronic properties of epitaxial single-layer NbS$_2$ on Au(111) — •Raluca-Maria Stan, Sanjoy Mahatha, Charlotte Sanders, Davide Curcio, Marco Bianchi, Philip Hofmann, and Jill A. Miwa — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark

In this study, the epitaxial growth of single layer NbS$_2$ on a Au(111) substrate has been achieved and techniques like scanning tunneling microscopy, low-energy electron diffraction, and angle-resolved photoemission spectroscopy have been used in order to investigate its structural and electronic properties. The excellent crystalline quality is revealed by the well-ordered hexagonal moiré superstructure and a well-defined orientation with respect to the Au(111) substrate. An accurate determination of the hexagonal lattice constant indicates agreement with the lattice parameter of the bulk parent compound. The electronic structure reveals two electron pockets crossing the Fermi level with appreciable broadening that can be due to hybridization with the substrate or strong many-body effects in the system. The metallic character has been shown and the general shape of the band structure is consistent with the 1H configuration. No indication of a charge density wave formation has been observed at a temperature down to 30 K.

O 66.5 Wed 17:45 Poster B2

Characterisation of MoS$_2$ and WS$_2$ demonstrating a general approach for the synthesis of two-dimensional binary compounds — •Ann Julie Holt[1], Raluca Maria Stan[1], Marco Bianchi[1], Abhay Shivayogimath[2], Philip Hofmann[1], and Timothy Booth[2] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus

C, Denmark — [2]DTU Nanotech, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

The synthesis of many two-dimensional materials is now scalable through different chemical vapor deposition (CVD) techniques. However, the crystal quality resulting from these methods is very sensitive to growth parameters and the details of the procedure are highly material-dependent. A significant amount of effort needs to be invested for the synthesis of each individual material, and the development of a general growth method would therefore be of great interest.

Here, we present an experimental study of two-dimensional single layer MoS_2 and WS_2 obtained from a general synthesis method developed for two-dimensional binary compounds. Structural and electronic characterization is performed by scanning tunneling microscopy (STM), low energy electron diffraction (LEED), and angle-resolved photoelectron spectroscopy (ARPES), showing high quality single-layer growth. These results serve as a proof of principle of a simple strategy for growing atomically thin binary compounds, which may greatly simplify the fabrication of already established and future two dimensional materials.

O 66.6 Wed 17:45 Poster B2

Growth and characterization of single layer tantalum phosphide compounds — •Federico Andreatta, Ann Julie U. Holt, Marco Bianchi, Jill A. Miwa, and Philip Hofmann — Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

Bulk transition metal pnictides have been recently found to host Weyl fermions, a novel state of topological quantum matter[1]. Transition metal pnictides are comprised of a transition metal and a group V element. Here, we show a method for growing tantalum phosphide compounds at the 2D limit on a Au(111) substrate. Using a combination of scanning tunneling microscopy and x-ray photoelectron spectroscopy we find two potential phases of single layer tantalum phosphide compounds. Intriguingly, one of the by-products of this growth method is single layer blue phosphorus[2]. We perform a systematic study of the growth parameters to tune the synthesis so that only single layer tantalum phosphide compounds are found at the surface.

[1] Z. K. Liu et al. Nat. Mater. (2015) 15, 27. [2] J. L. Zhang et al. Nano Lett. (2016) 16, 4903.

O 66.7 Wed 17:45 Poster B2

A Two-dimensional Sub-stoichiometric Molybdenum Sulfide with Catalytically Active Basal Planes — Yang Bao[1,2], Ming Yang[3], and •Kianping Loh[1] — [1]Department of Chemistry, National University of Singapore, 117543 Singapore — [2]TUM Fakultät für Physik, James-Franck-Straße 1, 85748 Garching bei München — [3]Institute of Materials Research and Engineering, 117602, Singapore

2D molybdenum disulfide (MoS2) has attracted immense interests recently due to its remarkable optoelectronic and catalytic properties. Other than the thermodynamically stable MoS2 structure, different metastable, sub-stoichiometric phases of MoSx (x<2) may exist due to the versatile Mo-S coordination, which may offer unique functionalities not seen in MoS2. While 0D [Mo3S13]2- cluster (Kibsgaards et al. Nat Chem 6, 248-253, 2014) and 1D Mo6S6 wire (Lin et al. Nat Nano 9, 436-442, 2014) have been reported, 2D phases of MoSx compounds are less well studied. Under-coordinated atoms in such 2D Mo-S polymorphs may give rise to periodic spin textures or chemically reactive surface sites.

Here we report the discovery of a 2D sub-stoichiometric MoSx (x<2) phase, where interesting structural features such as undercoordinated surface sites were clearly revealed by surface characterization techniques. Density function theory (DFT) studies suggest that 2D-MoSx may have a Mo18S18 unit cell. We have carried out catalytic studies on its basal plane and observed its ability to catalyze oligomerization of molecules as well as the activation of molecular hydrogen into atomic hydrogen.

O 66.8 Wed 17:45 Poster B2

Hematene for the oxygen evolution reaction — •Yidan Wei, Mahdi Ghorbani-Asl, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz Zentrum Dresden Rossendorf, Dresden 01328, Germany

Using density functional theory (DFT) calculations, the catalytic activity of a recent member of two-dimensional (2D) materials, hematene (α-Fe2O3 monolayer), has been studied for oxygen evolution reactions (OER). The stability and electronic structure of two experimentally faceted sheets of hematene, (001) and (010), was investigated. It was found that the (001) facet (1.589 eV) exhibits lower cleaving energy in comparison to the (010) facet (1.892 eV) suggesting a more stable structure. The electronic structure calculations indicate that facets of hematene for (001) and (010) are semiconducting monolayer with a large energy gap of about 1.51 eV and 1.36 eV in comparison to its bulk counterpart (1.8-2.2 eV). We also studied the relationship between the experimentally observed facets and their OER catalytic reactivity. It is found that the determining step in the OER process is the reaction of a H2O molecule in the surface to form an adsorbed hydroxyl group (O*). The variation of Gibbs energy is around 0.4 eV at most. The (010) facet showed a lower barrier for oxygen evolution than (001) facet. It was also demonstrated that the adsorption free energy and onset overpotential can be further tuned by defects, such as vacancies.

O 66.9 Wed 17:45 Poster B2

Oxygen interaction with h-BN on Ni(111) — •Christian Papp[1], Florian Späth[1], Soni Himadri[2], Fabian Düll[1], Johann Steinhauer[1], Udo Bauer[1], Philipp Bachmann[1], Hans-Peter Steinrück[1], and Andreas Görling[2] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen — [2]Friedrich-Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Chemie , Egerlandstr. 3, 91058 Erlangen

Hexagonal boron nitride (h-BN) is an interesting material to study, as an isoelectronic and structural analogue to graphene. However, due to the ionic character of the boron-nitrogen bond a bandgap of ~5.4 eV is found. This makes h-BN an interesting dielectric for graphene-based 2D-transistors. Moreover the band gap is ideal for emission of UV-light. To further modify the properties of 2D materials a chemical functionalization is needed.

In an activated adsorption process, molecular oxygen forms a molecularly bound species on a supported h-BN layer on Ni(111) at room temperature. By increasing the sample temperature to 400 K, oxygen can be intercalated under h-BN. At 600 K and higher, even the oxidation of h-BN becomes possible. The system was studied by XPS and NEXAFS. The results are supported by DFT calculations.

O 66.10 Wed 17:45 Poster B2

Layer dependent properties of quasi-freestanding 2H-TaS$_2$ investigated with STM and STS — •Camiel van Efferen[1], Joshua Hall[1], Clifford Murray[1], Matthias Rolf[1], Niels Ehlen[1], Jun Li[1], Jan Berges[2], Erik van Loon[2], Tim Wehling[2], Alexander Grüneis[1], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Theoretische Physik, Bremen Center for Computational Materials Science, Universität Bremen, Germany

We epitaxially grow quasi-freestanding TaS_2 multilayers on graphene on Ir(111) and investigate their thickness dependent properties up to three layers.

Using scanning tunnelling microscopy we observe the monolayer to be in the expected 3×3 charge density wave (CDW) phase, whereas the bilayer unexpectedly shows a 2×2 superstructure. Furthermore, the moiré of Gr on Ir(111) is no longer visible through the bilayer. Due to finite bilayer island sizes confinement effects occur, which interact with the superstructure.

We probe the electronic structure with low temperature scanning tunnelling spectroscopy, and find a strongly decreased density of states around the Fermi energy, as would be expected for a CDW. The width of the gap is compared with its monolayer analogue. We disentangle contributions from intrinsic bilayer properties, stacking effects and local confinement effects to the electronic structure.

O 66.11 Wed 17:45 Poster B2

Revealing the hydrogenated structure of silicene r13xr13 by STM tip induced dehydrogenation — •jinglan qiu — Hebei Normal University, Shijiazhuang, China

Although ordered and reversible hydrogenation has been demonstrated on silicene 4x4 and 2r3x2r3 superstructures, the hydrogenated structure of silicene r13xr13 (type I and type II) have not yet been revealed. Recently, we find that atomic hydrogen desorption processes can be induced by field-emitted or tunneling electrons from the STM tip, converting the hydrogen terminated silicene to intact monolayer silicene, including 4x4, 2r3x2r3 and r13xr13 phases. Bombardment of the surface with low energy (above 3eV) electrons desorbs the hydrogen and creates a bias dependent desorption area under the tip apex. From the high resolution STM images before and after hydrogen desorption, we get the one-to-one correspondence between hydrogenated silicene and various silicene phases. Interestingly, for silicene r13xr13 (type I), the hydrogenated structure appears almost identical to half-silicane that formed on silicene 2r3x2r3, indicating it an intact monolayer silicene as well. However, the hydrogenated structure of silicene r13xr13 (type II) shows quite differently with small pieces of silicene 1x1 surrounded by various size of black holes that expose the Ag(111) substrate. Thus, silicene r13xr13 (type II) should be regarded as a "precursor phase" for more ordered phases such as 4x4 and r13xr13.

O 66.12 Wed 17:45 Poster B2

The surface of high-temperature non-IPR fullerides — Jürgen Weippert[1], Seyithan Ulas[1], Eugen Wald[1], Bastian Kern[1], Dmitry Strelnikov[1], Mateo Amatti[2], Luca Gregoratti[2], Maya Kiskinova[2], and •Artur Böttcher[2] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — [2]Elettra, Sincrotrone Trieste, ScPA Area Science Park, 34149 Basovizza-Trieste, Italy

Alkali metal doped non-IPR fullerene materials C_n, $(n = 60 - 2k$ and $n = 70 - 2k$, $k = 1, ..5)$ represent a new class of fullerides.[1] We created Cs_xC_{58} and Cs_xC_{68} materials making use of the low energy cluster beam deposition (LECBD [2]). The non-IPR fullerene cages C_{58} and C_{68} form a covalently stabilized scaffold which gets doped by Cs atoms already during the growth. By heating the resulting material up to 1100K monodispersed high-temperature carbon solids, HT-Cs_xC_n, can be created. The resulting materials exhibit high stability and considerably depleted Cs contents. The carbon scaffolds are stabilized by multifold covalent intercage bonds.[3] The surface morphology is driven by on-top segregation in the two-component system. In both HT materials the surface topography is dominated by islands standing out by their elevated Cs/C_n ratio r.[1] Whereas the islands seen in Cs_xC_{58} exhibit r values not larger than 2 the bright surface areas in the Cs_xC_{68} solids surprise with extremely high r values (up to 70 Cs atoms per cage). [1] S. Ulas, et al. Phys. Status Solidi B 2018, 1800453 (1-13).[2] S. Ulas, et al. Carbon 2014, 68, 125-137.[3] S. Ulas, et al. J. Chem. Phys. 2012, 136, 114708.

O 66.13 Wed 17:45 Poster B2

Hydrogenation of bilayer graphene with excited H_2 — •Claus F. P. Kastorp[1], Anders L. Jørgensen[2], Martha Scheffler[1], John D. Thrower[1], David A. Duncan[3], Tien-Lin Lee[3], Liv Hornekaer[1], and Richard Balog[1] — [1]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [2]The Mads Clausen Institute, SDU NanoSYD, Sønderborg, Denmark — [3]Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, United Kingdom

Hydrogenation of single graphene layers provides a pathway for band gap tuning [1], while in bilayer graphene, functionalization could result in the formation of a diamane [2]. STM measurements show that bilayer islands grown by CVD on Ir(111) are not functionalized by excited H_2, but single layer areas are [3]. Similarly, no hydrogenation is expected for full bilayer graphene samples produced via MBE on Ir(111).

I will present standard XPS and hard X-ray standing wave photoemission experiments that show a high degree of hydrogenation in MBE grown bilayer graphene when exposed to excited H_2 molecules. Specifically, the components of the photoemission spectra that are associated with the bottom graphene layer, which is in direct contact with the iridium surface, indicate a level of hydrogenation that is comparable to the hydrogenation found for single layer graphene when exposed to excite H_2. The top layer component appears mostly unaffected.

[1] Balog, et al. Nature materials 9.4 (2010): 315.
[2] Leenaerts, et.al., Phys. Rev. B, 80.24 (2009): 245422.
[3] Hansen, L.K., Ph.D. thesis, Aarhus University (2017).

O 66.14 Wed 17:45 Poster B2

Sample preparation for Graphene Enhanced Raman Spectroscopy — •Stephan Sleziona, Simon Rauls, Leonard Christen, Tobias Foller und Marika Schleberger — Universität Duisburg-Essen, AG Schleberger, Germany

Graphene-enhanced Raman spectroscopy (GERS) has been shown to be a powerful tool for ultrasensitive detection of adsorbed molecules [1]. As a possible mechanism charge transfer is often suggested, which depends on the Fermi-level of the graphene, the HOMO-LUMO levels of the molecules and the excitation laser energy [2, 3]. Therefore, a combination of changing the fermi level in a graphene-based field effect device (GFET) and the excitation laser energy allows to investigate the coupling of this hybrid system. We prepared GFETs in two different ways: (i) with graphene grown by chemical vapor deposition (CVD) using photolithography and (ii) with exfoliated graphene using electron beam lithography (EBL). Cobalt Octaethylporphyrin (CoOEP) is deposited via thermal evaporation onto our substrates and the growth is analyzed using Raman spectroscopy and atomic force microscopy. Furthermore, we compare these fully processed samples with pristine samples to study possible influences of our lithography process on the various properties, such as graphene quality, molecular adsorption, and changes in the charge transfer mechanism of GERS.

[1] X. Ling et al., Small, 6 (2010), pp. 2020*2025
[2] E.B. Barros et al., Phys. Rev. B, 90 (2014), 035443
[3] Q. Hao et al., Appl. Phys. Lett., 102 (2013), 011102

O 67: Poster Wednesday: Solid-Liquid Interfaces

Time: Wednesday 17:45–20:00 Location: Poster B2

O 67.1 Wed 17:45 Poster B2

Structure of electric double layer at the graphene/ionic liquid interface probed by X-ray photoelectron spectroscopy — •Sunghwan Shin[1], Francesco Greco[1], Elmar Kataev[1], Olesya Kapitanova[2], Florian Maier[1], and Hans-Peter Steinruck[1] — [1]Friedrich-Alexander University Erlangen-Nürnberg, 91058, Erlangen, Germany — [2]Lomonosov Moscow State University, Leninskie gory, 119991 Moscow, Russia

Ionic liquids (ILs) electrochemical interfaces find applications in fuel cells, supercapacitors, and dye-sensitized solar cells. However, in situ analysis of these interfaces is difficult because of their inaccessibility to the surface science tools. Here, we report a photoemission study of electric double layer (EDL) formation on the graphene/IL electrolyte (1-methyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide) using a two-electrode electrochemical cell with graphene-covered porous silicon nitride membrane as a working electrode and a platinum wire as a counter electrode.

Cathodic and anodic polarization of graphene electrode up to 2V resulted in an asymmetric broadening of the peak in F 1s photoemission spectrum towards lower or higher binding energies correspondingly. For explaining this data, we developed a model consisting of EDL at the graphene/IL interface and a confined layer of IL situated between the graphene layer and the silicon nitride support and assign these shifts to the voltage drop at the working electrode.

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

O 67.2 Wed 17:45 Poster B2

Asymmetric Potential Screening at Electrode/Ionic Liquid Interfaces — •Sunghwan Shin, Francesco Greco, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie 2, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Ionic liquids (ILs) have received considerable attention as unique candidates to perform electrochemistry due to their larger electrochemical windows and high ion densities. To understand and control an electrochemical reaction in ILs, it is essential to understand the interface between ILs and metal electrodes playing a crucial role in capacitance charging and redox reactions. For ILs, potential screening (PS) at the anode and cathode interface can be dramatically different due to the asymmetric shape of the IL ions and their specific interactions with the charged electrodes. We studied PS effects by use of X-ray photoelectron spectroscopy (XPS) with an in situ two-electrode-cell. The amount of PS at the anode/cathode was determined using XPS binding energy shifts of the IL signals. In the case of symmetric Pt-Pt electrodes, the potential screening at the cathode was smaller than that at the anode for imidazolium-based ILs, which indicates a specific adsorption of imidazolium on platinum. For the Au-Au-setup, weak specific adsorption of imidazolium on gold leads to different PS effects that are related to the size of ions. Supported by the European Research Council (ERC) through an Advanced Investigator Grant to HPS (No. 693398*ILID)

O 67.3 Wed 17:45 Poster B2

First Principles Modeling of the Hydrogen Evolution Reaction in Mg Corrosion — •Tim Würger[1,2], Mikhail Zheludkevich[1], and Robert Horst Meissner[1,2] — [1]Helmholtz-Zentrum Geesthacht Centre for Materials and Coastal Research GmbH, Institute of Materials Research, Geesthacht, Germany — [2]Hamburg University of Technology, Institute of Polymer and Composites, Hamburg, Germany

Magnesium is a material with a high potential for a variety of applications in areas such as transport, energy and medicine. However, the corrosion properties of magnesium restrict its practical application and are still not fully understood. One unresolved phenomenon is the anodic hydrogen evolution, also called negative difference effect. High corrosion rates and corresponding hydrogen evolution are observed under anodic polarization, whereas fundamental corrosion concepts indicate hydrogen evolution to occur at the cathodic site. Iron replating is proposed to be a possible reason for the observed negative difference effect. In the corrosion process, embedded iron impurities are set free and replate on the magnesium surface where they promote the hydrogen evolution. As there is still no consensus about the preferred reaction site and mechanism of the hydrogen evolution, further investigations on an atomistic level in Mg as well as Fe systems are supposed to bring clarity. Obtaining further knowledge about the reaction energetics is crucial to find the favored hydrogen evolution site and mechanism, leading to a deeper understanding of magnesium corrosion and thus opening up new perspectives in magnesium corrosion engineering.

O 67.4 Wed 17:45 Poster B2

Study on femtosecond laser surface alloys for an improved catalytic activity — •Luise F. Hoffmann[1], Viktor Hoffmann[1], Matthias Koj[2], Andreas Gabler[1], Mia Börner[3], Anders Nilsson[3], Thomas Turek[2], Wolfgang Schade[1,4], and Thomas Gimpel[1] — [1]EST, Clausthal University of Technology, Goslar, Germany — [2]ICVT, Clausthal University of Technology, Clausthal-Zellerfeld, Germany — [3]Chemical Physics Division, Stockholm University, Sweden — [4]Fraunhofer Heinrich Hertz Institute, Goslar, Germany

Femtosecond laser material processing is used to alloy the surface structure of many materials. Chemical compositions are achieved far beyond conventional, thermal or metallurgical methods. Foreign substances in the substrate matrix help to tailor important material properties, such as the catalytic activity, the wettability, the heat transfer and fluid transport mechanisms. This is beneficial in order to functionalise electro catalysts e.g. for the electrochemical CO2 reduction reaction or the alkaline water electrolysis. However, the distribution of the additional elements is of main interest in order to evaluate the changed properties adequately. Therefore, energy dispersive x-ray spectroscopy as well as Auger electron spectroscopy is used to analyse the alloyed foreign substances in the structured substrate surface. We present studies on sulphur incorporated into copper and iron incorporated into nickel substrates. The composition is determined via cross-section images in spatial and depth resolution. This allows an extended understanding of the femtosecond laser material interaction.

O 67.5 Wed 17:45 Poster B2

Femtosecond laser iron incorporation of nickel electrodes for the alkaline water electrolysis — •Viktor Hoffmann[1], Luise F. Hoffmann[1], Matthias Koj[2], Thomas Turek[2], Wolfgang Schade[1,3], and Thomas Gimpel[1] — [1]EST, Clausthal University of Technology, Goslar, Germany — [2]ICVT, Clausthal University of Technology, Clausthal-Zellerfeld, Germany — [3]Fraunhofer Heinrich Hertz Institute, Goslar, Germany

The hydrogen production via alkaline water electrolysis is one of the key technologies for the energy transition. This technique will be used to store energy from fluctuating renewable sources. The chemical activity and microstructure are crucial factors determining the overpotential of an electrode within the electrolysis. Previous works show the enhanced efficiency of femtosecond laser structured electrodes in alkaline water electrolysis. In this work, iron is additionally incorporated into a nickel mesh electrode during the femtosecond laser treatment in order to improve the catalytic activity. Therefore, iron is provided from a liquid or a solid element source during the laser process. The influence of this treatment is analysed electrochemically. Furthermore, a scanning electron microscope with an energy dispersive x-ray spectroscope is used to characterise morphology and chemical composition of the electrode.

O 67.6 Wed 17:45 Poster B2

X-Ray photoelectron spectroscopic study of the near surface composition of [TfO] and [Tf2N] based Ionic Liquids at different electrode surfaces — Aleksandr Baranov, •Fabian Ullmann, Anna Dimitrova, and Stefan Krischok — Institut für Physik und IMN MacroNano, Technische Universität Ilmenau, Deutschland

With this contribution we will discuss the electronic structure and the ion assembly of four Ionic Liquids (ILs): 1-Ethyl-3-methylimidazolium trifluoromethanesulfonate ([EMim][TfO), 1-butyl-1-methylpyrrolidinium trifluoromethanesulfonate ([BMP]TfO), 1-ethyl-3-methylimida-zolium-bis-(trifluoromethylsulfonyl) imide ([EMim][Tf2N]) and 1-butyl-1-methyl pyrrolidinium-bis-(trifluoromethyl-sulfonyl)imide ([BMP][Tf2N]).

By using spin-coating technique and X-Ray Photoelectron spectroscopy we were able to prepare an IL*layers in *m and nm * range and to elucidate the chemical composition at the near surface and at the interface with three metal substrate: Ni, Ti and Au.

The results reveal that the cation/anion distribution depends on both: the IL used and the metal substrate. Moreover, a spectroscopic evidence demonstrate an existence of an anion*cation interaction, when TfO is present in the molecular structure.

O 67.7 Wed 17:45 Poster B2

Impact of the Electrolyte Salt Anion on the Solid Electrolyte Interphase (SEI) Formation at the Hard Carbon Electrodes of Sodium Ion Batteries — Gebrekidan Gebresilassie Eshetu[1,2,3], •Thomas Diemant[4], Maral Hekmatfar[1,2], Sylvie Grugeon[5], R. Jürgen Behm[1,4], Stéphane Laruelle[5], Michel Armand[3], and Stefano Passerini[1,2] — [1]Helmholtz Institute Ulm (HIU), Helmholtzstr. 11, D-89081 Ulm, Germany — [2]Karlsruhe Institute of Technology (KIT), P.O. Box 3640, D-76021 Karlsruhe, Germany — [3]CIC EnergiGUNE, Parque Tecnológico de Álava, Albert Einstein 48, E-01510 Miñano, Spain — [4]Institute of Surface Chemistry and Catalysis, Ulm University, Albert-Einstein-Allee 47, D-89081 Ulm, Germany — [5]Laboratoire de Réactivité et Chimie des Solides (LRCS) CNRS UMR 7314, Réseau Français sur le Stockage Électrochimique de l'Énergie (RS2E) FR CNRS 3459, F-80039 Amiens, France

Aiming at a more comprehensive understanding of the solid electrolyte interphase (SEI) in sodium ion batteries, we performed a detailed X-ray photoelectron spectroscopic (XPS) investigation of the few-nanometer thick passivation film formed on hard carbon (HC) in contact with various Na-ion conducting electrolytes (1M solutions of NaPF$_6$, NaClO$_4$, NaTFSI, NaFSI, or NaFTFSI in a 1/1 mixture of diethylcarbonate/ethylcarbonate). For comparison, analogous studies were carried out using LiPF6 and LiFSI as electrolyte salt. Taken together, the anion and cation of the electrolyte salt appear to play a key role for the overall SEI layer composition, including its depth evolution and thickness.

O 67.8 Wed 17:45 Poster B2

Electrolyte structure at Gallium Arsenide - KOH solution interfaces — •Alrik Stegmaier and Hans Hofsäss — 2. Physikalisches Institut, Georg-August Universität Göttingen

The electrolyte-semiconductor interface is a very active area of research. While the electrolyte structure near ideal surfaces in weak electrolytes are resonably well understood, non-ideal conditions, such as surface and near surface defects or strong electrolytes, are more difficult to understand. However, these conditions are important in many applications.

Here we present our latest results in modeling KOH solution structure near GaAs <100> surfaces with defects using molecular dynamics. For this we parameterize a polarizable force field against experimental, DFT, MP2 and CCSD(T) data. The electrolyte structure at different KOH concentrations and applied voltages is reconstructed. These results are compared against experimental data (such as impedance spectra) and continuum models.

O 67.9 Wed 17:45 Poster B2

Polarimetric angle-resolved second harmonic scattering on colloidal TiO2 nanoparticles in aqueous environments —

•Marie Bischoff, Arianna Marchioro, and Sylvie Roke — Laboratory for fundamental BioPhotonics (LBP), École Polytechnique Fédérale de Lausanne (EPFL), CH-1015, Lausanne

Titanium dioxide TiO_2 is a semiconductor material with a high physical and chemical stability. Therefore it is extensively studied for the use in environmental and energy applications, such as for example photocatalytic water splitting. Despite its highly promising characteristics, the underlying performance of TiO_2 is still limited. In order to enhance surface-mediated processes and photochemical reactions, it is crucial to understand the microscopic structure of the TiO_2/electrolyte interface.

Nonlinear optical techniques are powerful tools to study processes at surfaces and interfaces as they are sensitive to surface molecular orientation and interfacial electric fields. In this work we investigate TiO_2 nanoparticles in aqueous environments with nonlinear optical techniques, more specifically polarimetric angle-resolved second harmonic scattering (AR-SHS). We apply AR-SHS in order to extract information on the TiO_2/electrolyte interface and determine parameters such as surface potential and surface molecular orientation, which are difficult to obtain by other techniques.

O 68: Poster Wednesday: Nanostructures

Time: Wednesday 17:45–20:00 Location: Poster B2

O 68.1 Wed 17:45 Poster B2

Simulation of Brass Nanoparticles using a Neural Network Potential — •Jan Weinreich, Martín Leandro Paleico, and Jörg Behler — Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstr. 6, 37077 Göttingen, Germany

High-dimensional neural network potentials (HDNNPs) are a powerful method to study complex systems, because they offer the accuracy of density functional theory (DFT) calculations at the computational costs of simple empirical potentials thus enabling large-scale Monte Carlo and molecular dynamics simulations. In this work we construct a HDNNP for brass nanoparticles, which are important industrial catalysts for methanol synthesis. The potential is applied to determine the most stable structures of large brass clusters of varying composition and size. The analysis of the surface structures emerging in Monte Carlo simulations reveals that depending on the system size the copper to zinc ratio in the surface layers can strongly differ from the interior of the particles.

O 68.2 Wed 17:45 Poster B2

Iridium dioxide catalysts for water electrolysis - From Wulff shape to atomic structure and beyond — •Jakob Timmermann, Daniel Opalka, Christoph Scheurer, and Karsten Reuter — Technische Universität München, Germany

Iridium oxide is currently the preferred material to develop highly active and chemically stable nanoparticle catalysts for the electrochemical oxygen evolution reaction (OER) in proton exchange membrane electrolyzers. Computational models provide important support for the rational design of novel nanoparticle catalysts with optimal size, shape and stability. While the Wulff construction is often adopted to model single-compound nanocrystals, little is known about the influence of edge and corner atoms on the dimensional stability of ultra small IrO_2 nanoparticles as used in state-of-the art OER catalysts. In order to validate the inherent approximations of the Wulff construction, we compare relaxed, mono-facet IrO_2 Wulff nanoparticles of varying shape, size and stoichiometry to respective slab models for extended facets in a comprehensive structure analysis. We demonstrate that the geometry relaxation of IrO_2 nanoparticles strongly depends on the termination and, hence, thermodynamic parameters of the environment, prohibiting the application of the Wulff construction for certain IrO_2 surfaces. We further present an analysis of the contributions of facets, edges and corners to the surface free energy for selected nanoparticle models.

O 68.3 Wed 17:45 Poster B2

Cluster-surface interaction of plasmonic silver particles on silicon — •Katharina Engster[1], Kevin Oldenburg[1], Jean Lermé[2], Sylvia Speller[1], and Ingo Barke[1] — [1]University of Rostock, Institute of Physics, 18059 Rostock, Germany — [2]Université de Lyon, Institut Lumière Matière, 69622 Villeurbanne Cedex, France

Plasmonic nanoparticles interact with semiconductor surfaces in various ways. On the one hand the plasmon resonance is highly sensitive to the polarizable substrate on an atomic scale [1]. On the other hand plasmonically enhanced excitation of electron-hole pairs is expected to give rise to spatial variations of surface photovoltages (SPV), unless metallic surface states result in equilibration of the surface potential [2]. For size-selected Ag nanoparticles deposited on silicon we show that photoemission electron microscopy (PEEM) enables precise quantification of the SPV based on the spectrally resolved electron yield. The role of the plasmon resonance energy of individual particles, the detailed properties of the substrate (doping, surface states), and effects induced by the experimental setup are being discussed.

[1] K. Oldenburg et al., under review.

[2] K. Sell et al., Phys. Status Solidi B **247**, 1087-1094 (2010).

O 68.4 Wed 17:45 Poster B2

Growth and Morphology of Metal Clusters on HOPG — •christophe nacci[1], alexander schiffmann[2], Florian Lackner[2], Philipp Thaler[2], Wolfgang E. Ernst[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, 8010 Graz, Austria — [2]Institute of Experimental Physics, TU Graz, 8010 Graz, Austria

Clusters are a unique class of materials with extraordinary electronic, optical, and catalytic properties [1]. Gold nanoparticles are one of the most studied classes of nanoparticles due to their biocompatibility, high chemical and physical stability, the ease of surface functionalization with organic molecules and the optical properties related to surface plasmons. We have produced gold clusters by helium droplet synthesis and deposited them under clean ultrahigh vacuum (UHV) conditions onto an inert HOPG surface, where they were characterized by scanning tunneling microscopy (STM). Extended ramified structures were identified when depositing clusters on the surface kept at room temperature. In particular, the metallic structures exhibit a fractal-like pattern. The temperature dependence of their shapes has been explored by repeated post-deposition thermally annealing: A cross-over from fractal-like to smoother structures could be observed. To shed some light on the growth processes, Au clusters have been further deposited on an HOPG surface exhibiting defects created by ion sputtering in mild conditions.

[1] W. A. de Heer, Rev. Mod. Phys. 65, 611 (1993)

O 68.5 Wed 17:45 Poster B2

Manipulation of silver clusters in Ionic Liquids via added ligands. — •David Mönkebüscher, Alexander Kononov, Philippe Poulet, and Heinz Hövel — Fakultät Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany

Ionic Liquids (IL), e.g. BMIM-PF_6, delay the aggregation of nanoparticles due to their high viscosity and a formation of an ion layer around the clusters, which separates them electrosterically. Preformed silver clusters with an average size of 2 nm were deposited into different ILs [1]. The temperature dependent aggregation of the nanoparticles can be measured in-situ and ex-situ via UV/vis spectroscopy [2]. Ligands such as Dodecanethiole can be used to manipulate the aggregation of cluster due to the formation of a shell [3]. In order to investigate this influence, such mixed samples are compared with pure samples of different ILs. Another method to examine nanoparticles is AFM. It is used to detect silver clusters deposited on a MoS_2 surface to determine the cluster size distribution.

[1] D. C. Engemann, S. Roese, H. Hövel, J. Phys. Chem. C **120**, 6239 (2016). [2] S. Roese, A. Kononov, J. Timoshenko, A.I. Frenkel, H. Hövel, Langmuir **34**, 4811 (2018). [3] O. P. Khatri et al, Langmuir **24**, 7758 (2008).

O 68.6 Wed 17:45 Poster B2

Mass selected iron clusters on thin oxide films — •Kevin Foryt, Alexander Kononov, Dominik Wolter, and Heinz Hövel — Fakultät Physik/DELTA, Technische Universität Dortmund, 44227

Dortmund, Germany

Clusters are the bridge between atomic and solid-state physics, they show strong size dependent properties. In our cluster beam facility a magnetron sputter gas aggregation source produces a wide range of clusters. Mass selection is performed with a semicontinuous time-of-flight mass selector [1]. For deposition in a load-lock chamber attached directly to the mass selector a new setup of ion optics was simulated with SIMION [2] and has been put into operation. Iron clusters, e.g. $Fe_{1790 \pm 30}$, are deposited on an indium tin oxide (ITO) substrate which should be usable for magneto-optical studies. Afterwards ex situ UV/vis spectroscopy and AFM measurements are carried out.
[1] B. von Issendorff, R. E. Palmer, Review of Scientific Instruments **70**, 4497 (1999). [2] Scientific Instrument Services, Inc (2003-2012), http://simion.com.

O 68.7 Wed 17:45 Poster B2

An effective nanopatterning strategy for controllable fabrication of high-density sub-3-nm gaps — •Qun Fu[1,2], Huaping Zhao[1], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany — [2]Institute of Nanochemistry and Nanobiology, School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, China

The realization of large-scale high-density gaps with size as small as possible between neighboring nanostructures is crucial for designing ultrasensitive surface-enhanced Raman scattering substrates. As known, the ultra-thin alumina mask (UTAM) surface nanopatterning technique allows to fabricate large-scale (>1 cm2) ultrahigh-density (1010-1012 cm-2) 5-nm nanogaps in periodic nanostructure arrays. However, it is still difficult to realize reliable sub-5-nm gaps distribution on large area only by traditional one-step pore-widening process for UTAM technique, because of the collapse of the UTAM pore wall in the excessive pore-enlarge process at high operating temperature (30 C). Here, a two-step high-low temperature pore-widening process in the UTAM fabrication was reported as an efficient solution to precisely control the gap size into the range of sub-3-nm. This two-step pore-widening method enable to effectively avoid the fragmenting of the membrane and to obtain the large enough pore diameter to 97-99 nm steadily at appropriate lower temperature. As a result, large-scale nanoparticle arrays with high-density sub-3-nm gaps have been realized with the as-prepared UTAM as nanostructuring template.

O 68.8 Wed 17:45 Poster B2

Fabrication of metallic microstructures on optical fibers — •Alexander Fassbender and Stefan Linden — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

Fiber cavities have emerged to be a promising tool for the fabrication of a quantum memory cell. Based on the compactness and robustness of atom/ion traps that can be realized with fiber cavities, they are a candidate for the realization of quantum repeater nodes. We report on the fabrication of metallic microelements on optical fibers. A polymer mask is created on a cleaved end of the fiber using three-dimensional laser writing based on the principle of two photon absorption. A layer of gold is then thermally evaporated. After the removal of the polymer mask, four gold electrodes remain, separated by thin stripes that arise from the shadow of the polymer mask. The core of the fiber is protected as well, so the in- and outcoupling of light is not affected by the microstructures. When using these fibers in a cavity, the light-matter action can be manipulated. We envision that our microstructured fibers can be employed to realize compact ion traps inside of a fiber resonator.

O 68.9 Wed 17:45 Poster B2

Chemical properties of metal-silicates rendered by metal exchange reaction — •Franz Königer[2], Roberto C. Longo[1], Peter Thissen[2], and Alexei Nefedov[2] — [1]University of Texas at Dallas, Materials Science and Engineering 800 W. Campbell Road, RL 10 Richardson, TX, USA 75080 — [2]Karlsruher Institut für Technologie (KIT), Institut für Funktionelle Grenzflächen (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Calcium-Silicates and Calcium-Silicate-Hydrates (CS and CSH) form the most important building material, cement. Both phases react fast with CO2 from the atmosphere and, due to the porosity of cement and concrete, such reaction goes deep into the material, producing phase transformations and crack formation and propagation. The aim of this work is twofold. In the first part, we compare the reaction of CO2 with CSH phases and with Magnesium-Silicate-Hydrates (MSH). Surprisingly, MSH did not show any contamination of carbonates in the infrared spectra. While the reaction of CO2 with CSH has been well studied and explained, there is currently no explanation about the resilience of MSH to the interaction with CO2. For the first time, the atomistic details of the reaction of CO2 with MgSiO3 are shown, and the chemical resistance of MgSiO3 against CO2 and other relevant chemicals for corrosion of cement and concrete is explained. Secondly, we demonstrate that Mg and other metals can undergo an exchange in situ process in CS and CSH phases. Depending on the type of metal exchanged, a completely new platform for rendering the properties of cement and concrete surfaces against corrosion is developed.

O 68.10 Wed 17:45 Poster B2

Mechanism of SeOx2- Immobilization by δ-Bi2O3 Microsphere with Surface Oxygen Vacancies — •Long Liu[1], Huaping Zhao[1], Chenglin Zhang[1], Yang Xu[1], Dongjiang Yang[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany — [2]School of Environmental Science and Engineering, 266071 Qingdao, China

Removal of the toxic selenium compounds, e.g., selenite (SeO32-) and selenate (SeO42-), from contaminated water is imperative for environmental protection and drinking water safety. But conventional ion exchange and physical adsorption approaches are insufficient to achieve the required drinking water standard of selenium compounds with a concentration below 10 μg/L. Here we report that the preparation of microsphere-like δ-Bi2O3 with surface oxygen vacancies for efficiently capturing toxic SeOx2- (SeO32- and SeO42-) anions from aqueous solutions with superior capacity and fast uptake rate. The SeOx2- immobilization mechanism is attributed to the existence of surface oxygen vacancies, and implies the utilization of surface defects as highly efficient and adsorptive sites to capture specific toxic species.

O 68.11 Wed 17:45 Poster B2

Dielectric Waveguide Fabrication by Direct Laser Writing — •Frank Brückerhoff-Plückelmann, Alexander Fassbender, and Stefan Linden — Physikalisches Institut, Rheinische Friedrich-Wilhelms Universität Bonn, Nußallee 12, D-53115 Bonn, Germany

Direct laser writing allows the fabrication of three dimensional polymer structures from a negative tone photoresist by two photon absorption with an accuracy of a few hundred nanometer. By choosing the refractive index of the polymer slightly larger than the one of the glass substrate, we can use an external laser to excite guide modes in the printed structure [cf. Landowski, Freymann et al. '17]. For an efficient coupling we exploit the high refractive index difference between the polymer and air e.g. by designing a prism shaped coupler that uses total internal reflection at the polymer air interface. We study different coupler geometries and the overall performance of the polymer waveguides. In order to design larger optical networks we also test a simple beam splitting device.

O 69: Poster Wednesday: Organic Molecules on Inorganic Surfaces

Time: Wednesday 17:45–20:00 Location: Poster B2

O 69.1 Wed 17:45 Poster B2

Reactions of Tetrapyrroles with Lead on Metal Surfaces — •Mark Hutter[1], Malte Zugermeier[1], Guoqing Lyu[2], Martin Schmid[1], Stefan Renato Kachel[1], Nian Lin[2], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Department of Physics, The Hong Kong University of Science and Technology, Hongkong, China

Metal complexes of tetrapyrroles such as porphyrins and phthalocyanines play important roles in living organisms and for various technological applications. While most studies focus on transition metal complexes, we report here the interaction of tetrapyrrole monolayers with Pb as a typical main group metal. STM shows that tetrapyridylporphyrin (2HTPyP) on Au(111) reacts with metallic Pb, as evidenced by increased apparent heights in the molecular centers. Corresponding XPS studies with tetraphenylporphyrin (2HTPP) show the presence of Pb(II), indicating the formation of a Pb(II)TPP complex. Interestingly, annealing to 520 K leads to a reduction of the apparent height and the Pb(II) related XPS signal decreases. These findings are consistent with two possible mechanisms. In the first one, Pb(II)TPP is initially formed in a Pb-up geometry, such that the Pb(II) ion is detached from the Au substrate and thus retains its nominal oxidation state. Annealing transforms the complex to Pb-down geometry, in which the Pb(II) center receives electron density from the substrate and is reduced to Pb(0). In the second one, the Pb(II) center is replaced by a substrate Au atom upon annealing. For further clarification, TPD/AES studies were performed.

O 69.2 Wed 17:45 Poster B2

Rotation of a Single-Molecule Dipole — •Grant J Simpson[1], Víctor García-López[2], A. Daniel Boese[1], James M Tour[2], and Leonhard Grill[1] — [1]University of Graz, Graz, Austria — [2]Rice University, Texas, USA

Control of the orientation and the direction of rotation of a single molecule is crucial to the understanding of molecular machines. Directed rotation is also necessary to transfer mechanical work from one molecule to another in a controlled way. Here, we report how single dipolar molecules adsorbed on a Ag(111) surface can be oriented with maximum precision using the electric field in the junction of a scanning tunnelling microscope. Rotation is found to occur around a fixed pivot point and both directions of rotation are realised with 100% directionality. The pivot point arises as result of the interaction of an oxygen atom in the molecule and a silver atom of the surface. By introducing a further Ag adatom underneath the molecule, this interaction can be disrupted and the rotation of the molecule can be modified.

O 69.3 Wed 17:45 Poster B2

Investigation of side chain substituted quaterthiophenes on pristine and C_{60}-covered Ag(111) — •Jari Domke, Falko Sojka, Marco Gruenewald, Christian Zwick, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Side chain substituted dicyanovinyl quaterthiophenes (DCV4T-Et2) have been of interest for their application as absorber molecules in small molecule organic solar cells [1]. We investigate thin films of DCV4T-Et2 on Ag(111) as well as on C_{60} monolayers on Ag(111). Structural characterization of the films is carried out by means of distortion corrected low-energy electron diffraction (MCP-LEED) [2] and low-temperature scanning tunneling microscopy (LT-STM), optical characterization by differential reflectance spectroscopy (DRS) [3] and Photoluminescence (PL). We find that DCV4T-Et2 forms highly ordered structures on Ag(111). The optical properties depend on the layer thickness, most likely due to formation of aggregates.

[1] O. Guskova *et al.*, J. Phys. Chem. C **117** (33), 17285-17293 (2013).
[2] F. Sojka *et al.*, Rev. Sci. Instrum. **84**, 015111 (2013).
[3] R. Forker *et al.*, Annu. Rep. Prog. Chem., Sect. C: Phys. Chem. **108**, 34-68 (2012).

O 69.4 Wed 17:45 Poster B2

Spectroscopic studies of thin hemin and cytochrome-c films using a PEEM with fs-laser and He-I excitations — •Franz Niklas Knoop[1], Jonas Darius Fortmann[1], Ansgar Pausch[1], Klaus Stallberg[2], Gerhard Lilienkamp[1], Uwe Schröder[3], and Winfried Daum[1] — [1]IEPT, TU Clausthal — [2]Surface Physics, Uni Marburg — [3]IÖNC, TU Braunschweig

Microbial fuel cells (MFC) offer the potential to convert chemical energy of organics in waste water to electricity. Besides questions of technical realization, the electron transfer process in the bacterial biofilms is topic of current research. Previous studies suggest that redox-active, membrane-associated cytochromes play a crucial role in the transfer processes for Geobacter sulfurreducens, a promising candidate for MFCs. Aiming at a spectromicroscopic characterization of bacteria films, we studied thin films of the protein cytochrome c and the porphyrin hemin b, the latter being similar to the redox-active center heme c of the protein, using photoelectron emission microscopy (PEEM) with fs-laser excitation. For cytochrome c and hemin b we observe in our laser excitation spectra a pronounced Soret band at 415 nm and 400 nm, respectively, with very strong spectral broadening in the case of condensed hemin. While for cytochrome c laser-induced changes of the Soret band spectra were observed, hemin b spectra are not affected by laser irradiation. As a second route, we evaluate the possibilities of PEEM with excitation from a He-I UV light source and present first spectroscopic results for these films. We acknowledge financial support of the research group ElektroBak by the State of Lower Saxony.

O 69.5 Wed 17:45 Poster B2

Reorganization energy and polaronic effects in pentacene adsorbed on NaCl(001) surfaces — •Jakob Schlör, Daniel Hernangómez-Pérez, David A. Egger, and Ferdinand Evers — Universität Regensburg, Germany

Combined atomic-force and scanning-tunneling experiments allow to control single-electron transfer to and from organic molecules immobilized on electrically insulating NaCl surfaces [1]. By ramping the bias voltage, V_{bias} electrons tunnel in (out) of the molecule occupying the LUMO (HOMO) molecular orbital. V_{bias} at the onset of tunneling depends on the bias sweep direction, giving rise to a hysteresis that is closely related to the polaronic reorganization energy. Here, we employ electronic structure calculations based on the density functional theory to study the interplay of charging with ionic relaxations in the NaCl support. We calculate reorganization energies of different charge transitions for pentacene adsorbed on a NaCl(001)-surface and compare them to experimental findings.

[1] Fatayer et. al., Nature Nanotechnology, 13, p.376-380 (2018)

O 69.6 Wed 17:45 Poster B2

Electronic Structure and Interaction between Organic Charge-Transfer Molecules on Single-Layer MoS_2/Ag(111) — •Asieh Yousofnejad, Gaël Reecht, Christian Lotze, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Organic electronic devices such as organic solar cells and organic light emission diodes are highly promising devices for future technologies. Organic solar cells constitute electron donor (D) and electron acceptor (A) molecules for efficient charge separation upon photon absorption. At the interface between donor and acceptor, charge transfer may occur even without illumination. Using scanning tunneling microscopy and scanning tunneling spectroscopy, we study the structure and electronic properties of DCV5T-Me_2 (D) and C_{60} (A) on single-layer Molybdenum disulfide (SL-MoS_2) on Ag(111). SL-MoS_2 acts here as a decoupling semiconducting layer, which inhibits strong hybridization with the substrate. First, we investigate isolated islands formed by either C_{60} or DCV5T-Me_2. Co-depositing both molecules on MoS_2 also leads to homo-molecular islands. At the interface of C_{60} and DCV5T-Me_2 islands, we find a modified electronic structure, suggesting a charge transfer between C_{60} and DCV5T-Me_2.

O 69.7 Wed 17:45 Poster B2

Functionalization of Si(553)-Au surface with small organic molecules — •Sandhya Chandola[1], Julian Plaickner[1], Eugen Speiser[1], Conor Hogan[2], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften-ISAS- e.V. Schwarzschildstrasse 8, 12489 Berlin, Germany — [2]Istituto di Struttura della Materia-CNR (ISM-CNR), via Fosso del Cavaliere 100, 00133 Rome, Italy

The adsorption of small organic molecules on vicinal Au- Si(111) surfaces is shown to be a versatile route towards controlled growth of ordered organic-metal hybrid 1D nanostructures. We investigate molecular adsorption by establishing a direct connection between optical spectra and surface structure via ab-initio calculations. Optical spectra and their theoretical interpretation gives us information on structural and electronic properties of the system. We use a surface-sensitive and polarization-sensitive optical technique, Raman Spectroscopy (RS), to investigate the adsorption of toluene-3,4-dithiol (TDT) molecules on Si(553)-Au surfaces. As a first step, we use RS to investigate TDT adsorption on a SERS (surface enhanced Raman scattering) substrate which is known to produce significant surface enhancement when adsorbed with molecules. Distinctive vibrational modes have been identified and correlate well with the vibrational frequencies of the TDT molecule. RS of TDT adsorption on Si(553)-Au shows very weak vibrational modes which appear to be related to the molecular vibrations. In order to increase the detection sensitivity of the molecules on the Si(553)-Au surface, silver islands were deposited on the surface to increase the density of hot spots and thus enhance the Raman signal.

O 69.8 Wed 17:45 Poster B2

Formation of Highly Ordered Porous 2D Networks from Cyano-Functionalized Porphyrins on Cu(111) — •Rajan Adhikari, Michael Lepper, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

We investigated Cu-5, 10, 15, 20-tetrakis-(p-cyano)phenylporphyrin (CuTCNPP) on Cu(111) using Scanning Tunneling Microscopy in ultra-high vacuum at room temperature. While the adsorption behavior on Cu(111) in terms of intramolecular conformation and supramolecular arrangement of the free-base analogue 2HTCNPP and the corresponding porphyrin without cyano functionalization, i.e., CuTPP was previously reported, [1, 2] CuTCNPP behaves significantly different. It forms a peculiar hexagonal honeycomb-type pattern with triangular pores, initially coexisting with parallel arranged 1D molecular chains. Annealing to 400 K yields a complete transformation to the hexagonal honeycomb-type pattern. The hexagonal honeycomb pattern is formed by three Cu-TCNPP molecules linked by interstitial Cu-adatoms on the substrate. In summary, we report on a novel porous supramolecular structure, which might be well suited as a nanoscaled template. References: [1] M. Lepper, et al., Chem. Commun. 53 (2017) 8207 [2] K. Diller, et al., J. Chem. Phys. 136 (2012) 014705

O 69.9 Wed 17:45 Poster B2

Surface characterization of en-APTAS monolayers on n-GaN(0001) — •nurhalis majid[1,3], gerhard lilienkamp[1], nursidik yulianto[2,3], hutomo s. wasisto[2], and winfried daum[1] — [1]IEPT, TU Clausthal, Clausthal-Zellerfeld, Germany — [2]IHT, TU Braunschweig, Braunschweig, Germany — [3]Research Centre for Physics, LIPI, Tangerang Selatan, Indonesia

Surface functionalization of metal oxide semiconductors with N-[3-(trimetoxylsilyl)propyl]ethylenediamine (en-APTAS) self assembled monolayers provides a viable route for the development of selective NO2 gas sensors. A similar functionalization of GaN surfaces could allow for the development of nanoscale NO2 gas sensors. Here, we investigate properties of en-APTAS monolayers, prepared by dip coating on n-GaN(0001), by AFM, AES and XPS. The adsorption of en-APTAS is characterized by the SiLVV and SiKLL Auger lines and N 1s photoemission with binding energies of 398.8 eV, 400 eV, and 401.6 eV associated to primary, secondary and protonated amine groups, respectively. We observe an anomaly of the SiLVV/SiKLL Auger intensity ratio for the en-APTAS monolayer which suggests that the Si atoms are located close to the top of the layer. Implications for the suitability of this organic/inorganic hybrid system for NO2 gas sensing applications are discussed.

N. Majid would like to thank the Ministry of Research, Technology and Higher Education of the Republic of Indonesia for the Ph.D. scholarship and Indonesian-German Centre for Nano and Quantum Technologies for support.

O 69.10 Wed 17:45 Poster B2

Motorized molecules studied by scanning tunneling microscopy — •Peter Jacobson[1], James Tour[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, 8010 Graz, Austria — [2]Department of Chemistry, Rice University, Houston, Texas 77005, USA

Motorized molecules are envisioned as cargo carriers at the nanoscale. Critical to their success is the controlled activation of motion using external stimuli. In Feringa type motors, UV light triggers a sequence of isomerization and helical inversion steps leading to the unidirectional rotation of the motor. When incorporated into larger molecules, these motors are a potential source of unidirectional translation at surfaces. Scanning probe microscopy is an ideal tool to investigate the single molecule dynamics of these molecular machines, but commonly used metal substrates have drawbacks, such as the quenching of excited states by conduction electrons. An alternate approach is to deposit them on semiconducting substrates, thereby reducing the adsorption strength of the molecule on the surface and removing a potential path for quenching. Here, I will present initial results on motorized molecules containing a Feringa motor on semiconducting surfaces.

O 69.11 Wed 17:45 Poster B2

Superhydrophilic/hydrophobic double-sided polycaprolactone-based scaffolds produced via DC plasma treatment — •Ksenia Stankevich[1], Valeriya Kudryavtseva[1], Yuri Zhukov[2], Alexandra Pershina[3], Victor Filimonov[1], Evgeny Bolbasov[1], and Sergei Tverdokhlebov[1] — [1]National Research Tomsk Polytechnic University, Tomsk, Russian Federation — [2]Saint-Petersburg State University, Saint-Petersburg, Russian Federation — [3]Siberian State Medical University, Tomsk, Russian Federation

Polymer biodegradable scaffolds treated with plasma possess the essential properties of biocompatible materials. However, hydrophobic recovery occurring after the plasma treatment limits the application of the method. Here, we create thin porous polycaprolactone- (PCL-) based scaffolds with a thin Ti coating by direct-current plasma treatment. The plasma activated surface allows for the subsequent linker-free immobilisation of hyaluronic acid (HA) that helps to retain improved wettability. As HA is attached only to the plasma treated area of the material, a scaffold with a hydrophobic side and a superhydrophilic side can be created. Appropriate modification did not affect the morphology or mechanical properties of the scaffold, while improving scaffold wettability. The immobilised HA not only conferred high biocompatibility, but also stabilised the superhydrophilic surface against hydrophobic recovery. Cell proliferation assay demonstrated better cell adhesion to hydrophilic side modified with HA rather than hydrophobic. The proposed approach can potentially realise biomaterials with gradual wettability from biodegradable polymers.

O 69.12 Wed 17:45 Poster B2

Interfacial reactivity and adhesive properties of ternary transition metal nitride hard coatings in contact with polymers — •Martin Wiesing — Universität Paderborn, Paderborn, Germany

The surface oxidation behaviour of the prototypical nitric hard coating Ti0.5Al0.5N and its adhesive interactions with polycarbonate were investigated and related to its surface chemical and defect structure. The joint ion and electron spectroscopic analysis of the thermal and electrochemical surface oxidation allowed to develop a microscopic model of oxidation spanning the range from the early stages of oxidation to the formation of thick oxidation layers. The results corroborate the high significance of the surface electronic and defect structure for the reactivity of the metal-like and oxidic surfaces of Ti0.5Al0.5N.

UHV based Dynamic Force Spectroscopy (DFS) was performed to reveal the nature of the force interactions between Ti0.5Al0.5N and polycarbonate and their intimate relation to the surface oxide structure.

A novel experimental approach for the analysis of van der Waals forces based on Lifshitz theory combined with Reflection Electron Energy Loss Spectroscopy (REELS) was introduced to complement the force analysis. The method allows for the first time to determine highly accurate Hamaker coefficients of thin surface layers (>1 nm).

The here presented results are highly significant for understanding the corrosion and oxidation behaviour of hard coatings and to control their adhesive behaviour in contact with polymers.

O 69.13 Wed 17:45 Poster B2

Hybrid Zipper-Like Biopolymer Sorbents with Tunable Anion Sorption Properties — •Inimfon Udoetok[1], Lee Wilson[1], and John Headley[2] — [1]Department of Chemistry, University of Saskatchewan, 110 Science Place, Saskatoon, Saskatchewan, S7N 5C9 — [2]Water Science and Technology Directorate, Environment and Climate Change Canada, 11 Innovation Boulevard, Saskatoon, Saskatchewan, S7N 3H5

Quaternary composite (CGCFe) and ternary composite (CCFe) materials with variable morphology were prepared from carboxymethyl cellulose (CMC), chitosan, glutaraldehyde as the cross-linker, while iron III species acted as Lewis acid sites to impart unique anion binding properties. Characterization results provided evidence of cross-linking between the amine groups of chitosan and glutaraldehyde, variable iron doping and morphology for the composites. Equilibrium uptake results indicate that CGCFe surpassed the sorption capacity of CCFe, where greater uptake was noted at lower temperature. The monolayer sorption capacity of CGCFe for 2-naphthoxy acetic acid (S6) was 263 mg/g and 484 mg/g at alkaline and acidic pH conditions, respectively, with limited discrimination of OSPW naphthenate components, according to variable DBE or molecular weight range. Regeneration studies showed that CGCFe retained 95% of its sorption capacity after 5 cycles through a saline responsive zipper-like structural transition. This study provides insight on the role of Fe (III) species, cross-linking, and biopolymer structure that relate to anion binding properties in aqueous solution.

O 69.14 Wed 17:45 Poster B2

AFM as a unique tool for biological surface science: from collagen nanobiomaterials and cell guidance to cancer biomarkers and beyond — •Andreas Stylianou — Cancer Biophysics Laboratory, University of Cyprus, Nicosia, Cyprus

Atomic Force Microscopy (AFM) belongs to the scanning probe microscopy family and is one of the most popular techniques in surface science, including biological surface science and biomaterials. As the majority of biological interactions/reactions occur on surfaces or interfaces, it is of crucial importance to investigate the involved phenomena at the nanoscale level. In my talk, I will present the use of AFM as a unique tool in biological surface science based on my previous and ongoing research results. I will demonstrate the use of a number of AFM techniques in order to study (i) collagen thin film nanoscale formation and (ii) laser/optical radiation-collagen interactions [e.g., second harmonic generation (SHG), low level laser-(LLL) and ultraviolet-(UV)]. Furthermore, I will show how AFM can be used in order to investigate the effects of surface nanocharacteristics (nanotopography, nanomechanical properties) on cell-collagen interactions and how these characteristics guide cells, including their shape, orientation, mechanical properties and their migration/invasion properties. Finally, I will discuss recent and ongoing work aimed at using AFM techniques as a diagnostic tool for assessing cancer biomarkers for cancer cell identification, cancer diagnosis and therapeutic response prediction.

O 70: Poster Wednesday: Electronic Structure

Time: Wednesday 17:45–20:00 Location: Poster B2

O 70.1 Wed 17:45 Poster B2

Predicting Dirac semimetals based on Sodium Ternary Compounds — •Bo Peng — Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — Department of Optical Science and Engineering and Key Laboratory of Micro and Nano Photonic Structures (Ministry of Education), Fudan University, Shanghai 200433, China. — TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom.

Predicting new Dirac semimetals, as well as other topological materials, is challenging since the relationship between crystal structure, atoms and band topology is complex and elusive. Here, we demonstrate an approach to design Dirac semimetals via exploring chemical degree of freedom. Based on understanding of the well-known Dirac semimetal, Na3Bi, three compounds in one family, namely Na2MgSn, Na2MgPb and Na2CdSn, are located. Furthermore, hybrid-functional calculations with improved accuracy for estimation of band inversion show that Na2MgPb and Na2CdSn have the band topology of Dirac semimetals. The nontrivial surface states with Fermi arcs on the (100) and (010) surfaces are shown to connect the projection of bulk Dirac nodes. Most importantly, the candidate compounds are dynamically stable and have been experimentally synthesized. The ideas in this work could stimulate further predictions of topological materials based on understanding of existing ones.

O 70.2 Wed 17:45 Poster B2

Resolving the electronic surface structure of Lanthanum Hexaboride (001) — •Philipp Buchsteiner[1], Florian Sohn[2,3], Jan Voigt[1], Geetha Balakrishnan[4], Peter Blöchl[3,2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, 37077 Göttingen, Germany — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [3]Institut für theoretische Physik, Technische Universität Clausthal, 38678 Clausthal-Zellerfeld, Germany — [4]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

As Lanthanum Hexaboride (LaB6) is a wide-spread cathode material for electron emitters, its surface has been studied for a long time [1]. While Scanning Tunneling Microscopy (STM) has shown up to now a (1x1) reconstructed surface [2], only recently a (2x1) reconstruction has been predicted by theory to be the most stable (001)-surface structure [3]. Using UHV low-temperature STM and Scanning Tunneling Spectroscopy (STS) we have investigated the LaB6 (001) cleavage-plane. Our results confirm that atomically ordered surface areas are mostly labyrinth-like (2x1)-reconstructed. Combining STS and slab calculations within the framework of Density Functional Theory (DFT) allows us to further clarify the electronic structure, which is governed by 2pz-orbitals of the boron octahedra. This work is supported by the DFG grant WE1889/10-1 and PR298/19-1. [1] M. Trenary, Sci. Technol. Adv. Mater., 13 (2012) [2] J.S. Ozcomert, M. Trenary, Surf. Sci., 265 (1992) [3] K. M. Schmidt et al., Acta Mater. 144, 187-201 (2018)

O 70.3 Wed 17:45 Poster B2

Orbital surface reconstruction on SrTiO$_3$ studied with resonant x-ray reflectometry — •Benjamin Katter[1], Volodymyr Zabolotnyy[1], Eugen Weschke[2], Lennart Dudy[1], Ozan Kirilmaz[1], Sebastian Macke[3], Michael Sing[1], Ralph Claessen[1], Robert Green[4], and Vladimir Hinkov[1] — [1]Experimentelle Physik IV, Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany — [2]BESSY II, Helmholtz-Zentrum Berlin for Materials and Energy, 12489 Berlin, Germany — [3]Max Planck Institute for Metals Research, Heisenbergstraße 3, 70569 Stuttgart, Germany — [4]Department of Physics & Astronomy, University of British Columbia, Vancouver, B.C. V6T 1Z1, Canada

Transition metal oxides, like all crystalline solids, can show reconstruction effects at their surface due to breaking of the crystal symmetry. In titanium terminated SrTiO$_3$, in which the surface symmetry is lowered from O_h to D_{4h}, we observe a lifting of orbital degeneracy and shifting of orbital energies of Ti at the surface. To explore this, we have used Resonant X-ray reflectometry (RXR) to analyze orbital reconstruction at the surface of SrTiO$_3$ by combining surface and bulk sensitive reflectometry scans. We found a reconstructed surface layer of up to two unit cells in size where the optical constants of Ti were anisotropic. We fit and explain our results using crystal field theory.

O 70.4 Wed 17:45 Poster B2

Investigation of the electronic structure of triple-cations mixed-halides perovskites solar cell — •Sebastian Linke — Helmholtz-Zentrum Berlin, Berlin, Germany — Humboldt Universität zu Berlin, Berlin, Germany

In the past years perovskite solar cells have attracted a lot of attention with conversion efficiencies exceeding 22%[1]. One of the most promising perovskite materials is the mixed halides triple cations perovskites, which are used in some of the most efficient perovskite solar cells. In the inverted structure the backcontact is usually formed by PTAA layer on top of ITO substrates. The physical processes however are not fully understood yet. In particular, the interfacial energy level alignments are not addressed.

In this work, photoelectron spectroscopy (PES) is used to investigate the electronic structure of the individual layers, i.e. the PTAA and perovskite, separately. Then, the energy level alignment when forming the interfaces will be investigated, providing the information on the energy barrier of the charge carriers.

[1]Green et al.; Solar cell efficiency tables (version 52).; Prog Photo-

volt Res Appl. 2018;26:427*436.; https://doi.org/10.1002/pip.3040

O 70.5 Wed 17:45 Poster B2

Scanning Tunneling Spectroscopy on the f-electron system Praseodymium Hexaboride — •Lisa Harmsen[1], Philipp Buchsteiner[1], Geetha Balakrishnan[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, George-August Universität Göttingen, 37077 Göttingen, Germany — [2]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

The surfaces of f-electron systems like rare-earth hexaborides are prone to host correlation effects, such as heavy Dirac fermions [1]. While the Samarium Hexaboride surface have been studied in the past [2], only little is known about the electronic surface structure of the neighbouring f-electron system Praseodymium Hexaboride (PrB6). Here, we have investigated the (001)-cleavage plane of PrB6 with Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) down to 8 K. The acquired data reveals non reconstructed areas as well as several surface reconstructions. In contrast to Photoemission Spectroscopy measurements [3], where a large surface area is mapped, we are able to resolve the electronic structure locally including the local structure as seen in constant current topographies. This opens a way to disentangle f-electron physics on the atomic scale. This work is supported by the DFG grant WE1889/10-1 and PR298/19-1. [1] H. Pirie et al., arXiv:1810.13419 [cond-mat.str-el] (2018) [2] S. Rößler et al., Philos. Mag., 96:31, 3262-3273 (2016) [3] S. Patil et al., J. Phys.: Condens. Matter 23, 495601 (2011)

O 70.6 Wed 17:45 Poster B2

Experimental Growth and Characterization of Bi:CeAg$_x$/Ag(111) — •Hendrik Bostelmann-Arp, Katharina Kissner, Chul-Hee Min, and Friedrich Reinert — Julius Maximilians University of Würzburg, 97074 Würzburg

Recent theoretical studies point towards a new class of topologically non trivial materials, where the interplay of electronic correlation and strong spin orbit coupling is the driving force [1, 2]. Nevertheless, the existence of topological features in correlated systems has never been unambiguously clarified. Therefore, a first goal must be to realize materials in which both effects, spin orbit coupling and strong correlation, are observable. Very recently the influence of spin orbit coupling was reported in the substitution series Ce$_3$Bi$_4$(Pt$_{1-x}$Pd$_x$) ($0 \leq x \leq 1$), where the replacement of the heavier element Pt with the lighter Pd is suggested to induce a Kondo insulator to semimetal transition [3]. In this contribution we propose to merge electronic correlation and strong spin orbit coupling in the epitaxially grown surface alloy Bi:CeAg$_x$ on Ag(111). The surface lattice symmetry is determined by means of Low Energy Electron Diffraction. Furthermore, we investigate the changes in electronic dispersion as well as Ce 3d core level structure by Angle Resolved and X-Ray Photoelectron Spectroscopy. [1] M. Dzero, et al., Phys. Rev. Lett. 104, 106408 (2010) [2] J. Allen, Phil. Mag. 96, 3227 (2016) [3] S. Dzaber, et al., Phys. Rev. Lett. 118, 246601 (2017)

O 70.7 Wed 17:45 Poster B2

Fermi-Löwdin orbital self-interaction corrected DFT: application to phenolic acids — •Jakob Kraus, Sebastian Schwalbe, Torsten Hahn, and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany

The Fermi-Löwdin orbital self-interaction correction (FLO-SIC)[1] aims to counter the well-known self-interaction error (SIE) of density functional theory (DFT) in a computationally efficient and size-extensive way. FLO-SIC has been shown to reproduce the correct -1/r behavior of the potential as well as an adequate binding energy curve for stretched-bonds systems, a clear improvement over uncorrected DFT [2]. For selected phenolic acids, namely gallic acid and some of its derivatives, the bond-dissociation enthalpies (BDEs) as well as the ionization potentials (IPs) have been evaluated in the gas phase and in several test solvents. These molecular properties will be useful to predict a reaction path for the well-documented antioxidant properties of phenolic acids [3]. All results are presented as a comparison between uncorrected DFT and the most recent implementation of FLO-SIC DFT.

[1] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)
[2] S. Schwalbe et al., J. Comput. Chem., vol. 39, 2463 (2018)
[3] M. Nsangou et al., J. Mol. Struc., vol. 850, 135 (2008)

O 70.8 Wed 17:45 Poster B2

Vipster – A novel editor and visualization tool for periodic structures — •Sebastian Gsänger, Jonathan Gruber, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

When preparing structures for atomistic simulations or analyzing their results, one often has to decide between editing and visualization software. This is even more prevalent when dealing with periodic calculations, for which support has often been added to established programs as an afterthought. Here we present our endeavor to fill this gap with a portable and self-contained package that handles periodicity as a primary property. Utilizing modern platform-independent technology, we provide a featureful desktop client for all major operating systems, as well as a lightweight browser-based client and a scripting-interface via python.

O 70.9 Wed 17:45 Poster B2

PyFLOSIC: OpenSource implementation of Fermi-Löwdin orbital self-interaction corrected DFT — •Sebastian Schwalbe[1], Lenz Fiedler[1], Kai Trepte[2], Torsten Hahn[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, Germany — [2]Central Michigan University, Department of Physics, USA

We present the first developer version of the OpenSource implementation of the Fermi-Löwdin orbital self-interaction correction (FLO-SIC) [1,2] within the highly modular and modern PySCF code infrastructure. FLO-SIC aims to counter the well-known self-interaction error (SIE) of density functional theory (DFT) in a computationally efficient and size-extensive way, replacing the explicit solution of the N^2 localization equations with the optimization of $3N$ so called Fermi-orbital descriptors. The new implementation allows the usage of different unified Hamiltonians and is written in density matrix notation. These methodical changes allow the FLO-SIC method to be applicable on any functional implemented in the libxc library. Various examples for FLO-SIC applied to LDA-PW, the GGA functional PBE as well as the promising metaGGA SCAN functional will be discussed in detail.

[1] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)
[2] S. Schwalbe et al., J. Comput. Chem., vol. 39, 2463 (2018)

O 70.10 Wed 17:45 Poster B2

Proton uptake in the mixed ionic and electronic conductor BaFeO3-x — •Maximilian F. Hoedl, Rotraut Merkle, Eugene A. Kotomin, and Joachim Maier — Max Planck Institute for Solid State Research, Stuttgart, Germany

Many solid oxides containing oxygen vacancies can dissociatively absorb water leading to mobile protonic defects (hydroxide ions on oxide ion sites) in the lattice. The magnitude of water uptake appears to be determined by the basicity of the oxide ions in the solid. However, recent experimental studies suggest that in ionic-electronic mixed conductors such as BaFeO3-x perovskites, the water uptake can be disfavored by an interaction between protons and electron holes.[1] We present the results of first-principles DFT+U and HSE06 calculations on the interplay between the complex electronic structure and the water uptake in BaFeO3-x. The strong correlation effects of Fe3d electrons lead to a significant energy separation of spin-up and spin-down sub-bands. The spin-up band eventually falls below the O2p states and thus triggers a negative charge transfer from the oxide ions to the iron ions, creating holes in the O2p valence band. This reduces the negative charge on the oxide ions and the oxide ion basicity. The calculated hydration enthalpies depend on the hole concentration varying between zero for BaFeO3 and about -1 eV for BaFeO2.6. [1] R. Zohourian et al., Adv. Funct. Mater. 2018, 28, 1801241

O 71: Poster Wednesday: Adsorption and Catalysis

Time: Wednesday 17:45–20:00 Location: Poster B2

O 71.1 Wed 17:45 Poster B2

Synthesis on surfaces: direct desulfurization and hyperthermal reactions of Reichardt's dye — •Tomasz Michnowicz[1], Bogdana Borca[1,2], Rémi Pétuya[3], Marcel Pristl[1], Ulrike Kraft[1], Hagen Klauk[1], Pavel Jelinek[4], Andres Arnau[3], Uta Schlickum[1,5], Lukas Krumbein[1], Suman Sen[1], Martina Stella[6], Andrea Floris[6], Allesandro de'Vita[6], Stephan Rauschenbach[1,7], and Klaus Kern[1,8] — [1]Max Planck Institute for Solid State Research, Germany — [2]National Institute of Materials Physics, Romania — [3]UPV/EHU San Sebastian, Spain — [4]Insitute of Physics CAS, Czech Republic — [5]TU Braunschweig, Germany — [6]King's College, UK — [7]University of Oxford, UK — [8]École Polytechnique Fédérale de Lausanne, Switzerland

We present combined STM/AFM studies of molecular structures acquired via two different approaches to on-surface chemical reactions: local, precise control of a desulfurization process and a kinetically induced reaction of Reichardt's dye. The first reaction is driven by the local electric field present in the STM tip-sample junction. We demonstrate the subsequent dissociation of both carbon - sulfur bonds of a thiophene group embedded in tetracenothiophene (TCT) molecules on Cu(111). For the second system we utilize the Electrospray Ion Beam Deposition (ES-IBD) to collide single molecular ions of Reichahrdt's dye with a Cu(100) surface at energies in the hyperthermal regime. With this technique, new species of Reichhardt's dye can be obtained (e.g. including ruptured benzene rings), inaccessible by means of a standard thermal activation path.

O 71.2 Wed 17:45 Poster B2

Model catalytic studies of liquid organic hydrogen carriers: Indole/Indoline/Octahydroindole on Ni(111) — •Johann Steinhauer, Philipp Bachmann, Udo Bauer, Fabian Düll, Florian Späth, Hans-Peter Steinrück, and Christian Papp — Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen

The availability of energy from renewable sources is unsteady and unpredictable due to environmental influences. Therefore, energy storage becomes more important in the near future. One route to store energy in the form of hydrogen are liquid organic hydrogen carriers (LOHCs) that enable chemical storage of hydrogen. In an LOHC system, organic molecules are catalytically loaded with hydrogen to form an energy- and hydrogen-rich compound. Afterwards, hydrogen is catalytically unloaded. Recent studies identified the N-based heteroalicyclic system N-ethylcarbazole (NEC) as suitable LOHC (hydrogen capacity of 5.8 wt%). Herein, we present detailed studies on the LOHC system indole, with the hydrogen-rich octahydroindole (hydrogen capacity of 6.4 wt%), the dehydrogenation intermediate indoline and the hydrogen-lean indole. This system is investigated in a model approach on a Ni(111) surface under ultra-high vacuum conditions. HR-XPS and TPD are used to provide insights in the adsorption, desorption and reaction behavior of the LOHC system. We will present a detailed description of the reaction pathway and discuss the use of this system for chemical hydrogen storage. A comparison and evaluation of the differences to the known system H12-NEC / NEC will be presented.

O 71.3 Wed 17:45 Poster B2

A confined hydrogen molecule chopping light emission from a tunnel junction — Pablo Merino[1,2,3], Anna Rosławska[1], Christopher C. Leon[1], Christoph Grosse[1], César González[4], •Klaus Kuhnke[1], and Klaus Kern[1,5] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Instituto de Ciencia de Materiales de Madrid, Spain — [3]Instituto de Física Fundamental, Madrid, Spain — [4]Departamento de Física Teorica de la Materia Condensada, Madrid, Spain — [5]École Polytechnique Fédérale de Lausanne, Switzerland

We combine scanning tunneling microscopy (STM) with optical correlation spectroscopy to access the dynamics of H_2/Au(111). At low coverage (ca. 2%) molecular hydrogen forms a hexagonal superlattice with a large intermolecular spacing of 2 nm ascribed to molecular interaction dominated by surface state electrons at the Fermi energy. We characterize this yet unexplored glassy phase which provides an open structure in which a single molecule is confined - yet free to move in and out of the tunnel junction. Plasmonic light emission from the STM junction in constant height mode is employed to observe this motion by means of the resulting intensity modulation. Analyzing the time-resolved photon train detected in the far-field provides an autocorrelation function $g^{(2)}(\Delta t)$ which is dominated by one exponential. The residence time in the junction (10 ms) and the out-of-junction excursion time (3 ms) are obtained by modeling the system with a two-state (in-junction ⇔ out-of-junction) rate equation model.

O 71.4 Wed 17:45 Poster B2

Moving atoms on surfaces: The impact of external parameters on the required force — Jonathan Brand, •Nicolas Néel, and Jörg Kröger — Technische Universität Ilmenau, Ilmenau, Germany

Combining scanning tunneling microscopy and atomic force spectroscopy the dependence of the lateral force to move single adsorbed atoms on surfaces on the temperature is explored. A decrease of the force with increasing temperature is observed for all atoms and surfaces investigated and may be captured in a simple model. Crossing the critical temperature as well as surmounting the critical magnetic field of a superconductor does not lead to discriminable changes in the lateral force.

O 71.5 Wed 17:45 Poster B2

Addressing individual redox states of single polyoxovanadate molecules — •Marco Moors[1], Oliver Linnenberg[2], and Kirill Yu. Monakhov[3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Wilhelm-Johnen-Straße, 52425 Jülich — [2]Institut für Anorganische Chemie, RWTH Aachen, Landoltweg 1, 52074 Aachen — [3]Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig

Polyoxometalates (POM) offer a great potential for future applications in the fields of catalysis, sensors or molecular data storage. An outstanding property of POM consisting of vanadium ions is the ability of the latter to transit between multiple stable redox states, without affecting the structural integrity of the molecule [1]. In this study we present a model approach for tailoring and testing tris(alkoxo)-terminated Lindqvist-type POM as operational units for (multi-)resistive switching memories. This POM class is characterized by a rather small negative molecular charge of its fully-oxidized species and can be easily derivatized with different organic ligands. By applying an external potential we were able to demonstrate the controlled addressing of individual redox states of a single molecule adsorbed on an Au(111) surface at room temperature [3].

[1] K. Y. Monakhov et al., Adv. Inorg. Chem. 69 (2017) 251; [2] D. Li et al., J. Am. Chem. Soc. 133 (2011) 14010; [3] O. Linnenberg et al., J. Am. Chem. Soc. DOI: 10.1021/jacs.8b08780 (2018).

O 71.6 Wed 17:45 Poster B2

Epiminotetracenes on Au(111) — •Frank Eisenhut[1,2], Dmitry Skidin[1,2], Fátima García[3], Diego Peña[3], Gianaurelio Cuniberti[1,2,4], and Francesca Moresco[1,2] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [3]Centro de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS) and Departamento de Química Orgánica, Universidade de Santiago de Compostela, 15782-Santiago de Compostela, Spain — [4]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

The introduction of substituents into the aromatic core has been proven to be a versatile tool in the generation of acenes. Within this study, we use a tetracene precursor with two embedded epiminogroups in the aromatic backbone, wehreas after moderate annealing one nitrogen-carbon bond can be cleaved or the complete group can be dissociated. This partial reaction has been proven with high-resolution STM images. While we could verify that the originated tetracene molecules with two of these new formed groups are strongly bonded to the surface and cannot be manipulated, we could show that the molecules with one nitrogen-containing side group after the reaction can be rotated around the nitrogen atom. Consequently, the molecules are anchored on Au(111) with nitrogen-gold bonds via the emerging side groups after the planarization and breaking of the bond.

O 71.7 Wed 17:45 Poster B2

Anchoring strategies for a molecular gear on Au(111) — •Tim Kühne[1,2], Frank Eisenhut[1,2], Jorge Monsalve[1,2], Claire Kammerer[3], Gianaurelio Cuniberti[1,2,4], and Francesca Moresco[1,2] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [3]CEMES, Université de Toulouse, CNRS, Toulouse, France — [4]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

A fundamental component of a planar single-molecule mechanical machine is a molecular gear, whose construction needs a proper combination of the molecular design, a smart selected surface for anchoring as well as the controlled rotation by manipulation. We investigated the adsorption of single pentaphenylcyclopentadiene molecules (PPCP) on Au(111) by LT-STM. We took advantage of the radical character after the tip-induced dehydrogenation of the single hydrogen at the cyclopentadiene core and studied the step-by-step rotation of this species using the lateral manipulation mode. As a last approach, we positioned PPCP on gold atoms and -clusters to examine the usage of these clusters as gear wheel axles.

O 71.8 Wed 17:45 Poster B2

Hydrogenation of ethylene on supported size-selected Pt-clusters — •Kevin Bertrang, Maximilian Krause, Marian Rötzer, Andrew Crampton, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstraße 4, 85748 Garching, Germany

The interplay between catalyst and support, e.g. thin silica films on metal single crystals, has proven a key factor in the activity of such systems. The nature of their interaction determines the charge transfer to the supported catalyst and therefore its electronic proprieties. The catalyst's local electron density can be altered by varying the underlying metal, which allows to tune the reactivity of the catalyst by specifically (de)charging it. Additionally to the bonds formed at the metal-silica interface, the resulting local work function of the support was found to govern charging effects. A system exhibiting a high local work function yields cluster of positive partial charge, vice versa clusters are partially charged negative with a low local work function. In this context, the change in activity of size-selecteed Pt-clusters towards ethylene hydrogenation has been investigated under steady-state conditions supported on thin silica films on different metal single-crystals. The catalytic samples were characterized through TPD, IRRAS and electron spectroscopy.

O 71.9 Wed 17:45 Poster B2

Effect of molecular structures on Metathesis reaction and its potential application — •Xiangzhi Meng[1,2], Lacheng Liu[1,2], Fatima Garcia[3], Berta Alvarez[3], Dolores Perez[3], Hong-Ying Gao[1,2], Diego Pena[3], and Harald Fuchs[1,2] — [1]PhysikalischesInstitut,WestfalischeWilhelms-UniversitaẗMünster,Wilhelm-Klemm-Straße10,48149Münster,Germany — [2]Center for Nanotechnology, Heisenbergstraße 11, 48149 Münster, Germany — [3]CentrodeInvestigacioń enQuímicaBioloxicaeMateriais-Moleculares(CIQUS)andDepartamentodeQuímicaOrgańica, Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain

Recently, the σ-bond metathesis reaction has been reported between aromatic silylated alkynes and carboxylic acids on metal surfaces. Here, we further studied the effect of the molecular structures on the metathesis reaction on different (111) surfaces. Two silylated tetraynes with nonaromatic alkene and aromatic naphthalene as central cores were prepared and tested together with aromatic acids. A low-temperature scanning tunneling microscope was used. We found the aromatic tetrayne has a higher reactivity in the metathesis reaction than the nonaromatic tetrayne. It is also found that the metathesis reaction is surface-dependent. The metathesis reaction could become a new method for the bottom-up strategies and the related discoveries here will open new doors for the molecular designs in on-surface reactions.

O 72: Poster Wednesday: Scanning Probe Techniques

Time: Wednesday 17:45–20:00 Location: Poster B2

O 72.1 Wed 17:45 Poster B2

The Use of Spherical Particles for Cantilevers in an Atomic Force Microscope — •Katja Stommel, Hsiao-Ching Tsai, and Mathias Getzlaff — Institut für Angewandte Physik, Heinrich-Heine Universität Düsseldorf, Germany

The elasticity of cells is an important property and mainly influenced by the cell's cytoskeleton. With an AFM it is possible to measure the elasticity of soft materials. It is necessary to use a probe tip with a known, well-defined shape to determine the Young Modulus of, e.g., cells using the Hertz model. Hence, the goal of this project is to test and document a reproducible method of attaching a spherical particle to a cantilever.

A combined system including an AFM and a transmitted light-microscope is used for the process, during which a spherical particle of silica is glued at a tipless cantilever. To control the quality of the modified cantilever, another transmitted light-microscope is used. Images showing the side and the top view are acquired and used to determine the size and shape of the attached particles. The quality check shows that the method to modify cantilevers cannot be reproduced easily. Because the imaging is not precise enough, the conditions of the Hertz model are not necessarily fulfilled.

O 72.2 Wed 17:45 Poster B2

Upgrade of a low-temperature STM for single atom electron spin resonance — •Fabian D. Natterer[1,2], François Patthey[1], Tobias Bilgeri[1], Patrick R. Forrester[1,2], Nicolas Weiss[1], and Harald Brune[1] — [1]Institute of Physics, EPFL, Lausanne, Switzerland — [2]Physik-Institut, University of Zurich, Switzerland

Electron spin resonance with a scanning tunneling microscope (ESR-STM) combines temperature independent energy resolution in the nano-electron range and control of the atomic dimensions. We describe here the transformation of a low-temperature STM to an ESR-STM. The system is capable of delivering RF power to the tunnel junction at frequencies up to 30 GHz. We perform ESR on the model system TiH/MgO/Ag(100) by sweeping the magnetic field and find a magnetic moment of $(1.004 \pm 0.001)\ \mu_B$. Our upgrade enables to toggle between a DC mode, where the STM is operated with the regular control electronics, and an ultrafast-pulsed mode that uses an arbitrary waveform generator for pump-probe spectroscopy or reading of spin-states. Both modes allow for simultaneous radiofrequency excitation, which we add via a resistive pick-off tee to the bias voltage path. The RF cabling from room temperature to the 350 mK stage has an average attenuation of 18 dB between 5 and 25 GHz. Additional losses occur at the flexible cable segment connecting the STM tip. We discuss our transmission losses and indicate ways to reduce attenuation. We finally demonstrate how to synchronize the arrival times of RF and DC pulses coming from different paths to the STM junction, a prerequisite for future pulsed ESR experiments.

O 72.3 Wed 17:45 Poster B2

Analysis and quantification of electrochemical strain in contact resonance atomic force microscopy — •Sebastian Badur, Thomas Göddenhenrich, and André Schirmeisen — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392

Contact resonance atomic force microscopy can be used to measure the electrochemical strain caused by ionic movement (Vegard strain).

These potential-induced local surface deformations strongly depend on ionic concentration, electric field distribution and diffusion time. Besides that, local electrochemical strain response is mostly superimposed by other local tip-sample contact mechanics from local and non-local electrostatic forces that contribute to the image contrast formation.

For measuring and quantifying electrochemical strain, we developed a method to eliminate these parasitic contributions by using band excitation in a low and high frequency regime of the cantilever excitation.

As sample, we use Li_xCoO_2 as a typical battery cathode material. Contact resonance measurements and additional current measurements were done with conductive cantilevers and tips under UHV condition.

O 72.4 Wed 17:45 Poster B2

Design of a New Photon Collecting STM — •Mike Stummvoll[1], Markus Etzkorn[1], and Uta Schlickum[1,2] — [1]Technische Universität Braunschweig, Institut für Angewandte Physik, Mendelssohnstr. 2, 38106 Braunschweig — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

To access dynamical properties of single photon sources on surfaces, atomic scale control is mandatory. For the improved characterisation of charge carrier and exciton dynamics, we design a new scanning-tunnelling microscope (STM).

The tunnel current in an STM tunnel junction can be used to excite photons locally on atomic scale objects. To collect the emitted photons we will employ a parabolic mirror, which will be aligned *in-situ* using piezo-driven actuators. An external optical set-up will be used for optical analysis. A spectrometer will yield information on the photon wavelength while avalanche photo-diodes (APDs) will be used for single-photon detection and high time resolution.

O 72.5 Wed 17:45 Poster B2

The Kondo resonance line shape in scanning tunnelling spectroscopy: instrumental aspects — •Manuel Gruber, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

The differential-conductance spectrum of magnetic adsorbates on surfaces can exhibit a zero-bias feature originating from the many-body Kondo effect. The intrinsic line shape of this Kondo resonance and its temperature dependence contain, in principle, valuable information. In the present study, using low-temperature scanning tunneling microscopy along with model calculations, we investigate the influence of instrumental broadening on the Kondo line shape of a model molecular Kondo system (all-*trans* retinoic acid on Au(111)). The modulation voltage used for the lock-in detection, noise on the sample voltage, and the temperature of the microscope tip are considered [1].

This work was supported by the DFG through SFB 677 and the European Union's Horizon 2020 research and innovation programme under grant agreement No. 766726.

[1] M. Gruber, A. Weismann, R. Berndt, J. Phys. Condens. Matter **30**, 424001 (2018)

O 72.6 Wed 17:45 Poster B2

Apparent tunneling barrier height and local work function of atomic arrays — Neda Noei, Alexander Weismann, and •Richard Berndt — IEAP, CAU Kiel, D-24098 Kiel

Spatially resolved measurements of the apparent tunneling barrier height $\Phi_{\rm app}$ in scanning tunneling microscopy have been used to estimate variations of the local work function Φ of surface structures. We experimentally show that $\Phi_{\rm app}$ can fail as a measure of Φ. The discrepancies are attributed to a kinetic energy contribution to $\Phi_{\rm app}$. This contribution depends on the lateral extent of the tunneling current filament and, consequently, on the local surface structure. Support by DFG via SFB 677 is acknowledged.

O 72.7 Wed 17:45 Poster B2

Design of a low-temperature scanning tunneling microscope for detection of single-molecule light emission — •Tzu-Chao Hung, Brian Kiraly, Alexander A. Khajetoorians, and Daniel Wegner — Radboud University, Institute for Molecules and Materials (IMM), 6500 GL Nijmegen, The Netherlands

Phosphorescent triplet-emitter molecules are promising candidates for highly efficient OLEDs, but it is not well understood how the optoelectronic properties are altered when they are embedded in a device environment. In order to fundamentally study such dependences with atomic-scale resolution, we upgraded a low-temperature STM (T= 4K) to detect tip-induced light emission from the tunnel junction. An insitu lens is placed close to the tunnel junction to collimate the light out of the ultrahigh vacuum system into a fiber coupler. The end of the fiber is either guided to a spectrometer with an LN2-cooled CCD detector or to a single photon counting module. This way, we are able to simultaneously study the structure, electronic properties and light-emission spectra of single molecules down to submolecular resolution and with photon yields down to few counts per second. We will present the design and performance of the setup and show preliminary results on single-molecule light emission of ZnPc molecules.

O 72.8 Wed 17:45 Poster B2

Contrast mechanism in Scanning Field Emission Microscopy — •Gabriele Bertolini[1], Robin Pröbsting[1], Hugo Cabrera[1], Urs Ramsperger[1], Danilo Pescia[1], and Oguzhan Gürlü[1,2] — [1]Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland — [2]Istanbul Technical University, Department of Physics, 34469 Istanbul, Turkey

We perform Scanning Tunneling Microscopy in the field emission regime by retracting the tip few nanometers away from the sample, out of the tunneling condition. By applying a higher negative potential to the tip with respect to the sample, field emission of electrons is achieved. Formally this technique is named as Scanning Field Emission Microscopy (SFEM) and it is based on STM in combination with Topografiner technology. SFEM can provide chemical and magnetic information of surfaces with nanometer level spatial resolution due to the high sharpness of the tip. During experiments we simultaneously measure the amount of emitted electrons from the tip, the absorbed electrons by the sample, as well as the electrons escaping the tip-sample junction. In our setup we also have an electron energy analyzer. In this work we present our results on the chemical contrast observed in different metal and semiconductor surfaces as well as metal/semiconductor interfaces using SFEM. We show how the contrast mechanism observed on the current and electron maps of the surface can be interpreted and can be enhanced.

O 72.9 Wed 17:45 Poster B2

Collection and Detection Mechanisms for Photons Emerging from Tunnel Junctions — •Berk Zengin[1,2], Hugo Cabrera[2], Dilek Yildiz[2,3], Danilo Pescia[2], and Oguzhan Gürlü[1,2] — [1]Istanbul Technical University, Department of Physics, 34460, Istanbul, Turkey — [2]ETH Zurich, 8093, Zurich, Switzerland — [3]University of Basel, Basel, Switzerland

Even though photon emission from planar tunneling junctions were studied long before the invention of Scanning Tunneling Microscope (STM), studies on such photon generation mechanisms are gaining more interest in recent years. Several photon collection and detection mechanisms with high efficiencies were reported. We constructed several photon collection mechanisms on a commercial STM system. In one, emitted photons were collected using a fiber that was placed in proximity of tunneling junction, mounted on a manual positioner. Based on simulations carried out by finite element methods, a ball lens was placed in between fiber and the junction to increase coupling efficiency and results were compared accordingly. Furthermore, a bundle of two fiber cores were used to detect photons in order to perform two channel photon detection from the tunnel junction. Two types of detectors were utilized for photon collection process. Our results indicate that photon maps acquired simultaneously with topography and tunneling current maps can show contrast between neighboring data points, demonstrating a resolution with several Angstroms. In general, we address the challenges of interpretation of photon maps obtained under ambient conditions due to changes at the tip apex.

O 72.10 Wed 17:45 Poster B2

A Time and Spatially Resolved Study of the Thermal Response of the Tip of a Scanning Tunneling Microscope on Pulsed Optical Excitation — •Georg Alexander Traeger[1,3], Taner Esat[1,2], Martin Wenderoth[3], and Jungseok Chae[1,2] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul, Republic of Korea — [2]Department of Physics, Ewha Womans University, Seoul, Republic of Korea — [3]IV. Physics Institute, Georg- August-University, Göttingen, Germany

Combining Scanning Tunneling Microscopy (STM) and pulsed optical excitation was already envisioned in the early 1990s. [1] In this approach, disentangling thermal effects due to heating of the tip from optically induced dynamics of the sample has always been a major issue. Grafström et al. [2] sytematically investigated the thermal response on sinusoidal stimulus up to 100 kHz. Only recently, Kloth et al. [3] estimated thermal effect of pulsed optical excitation based on the shaken pulse pair excitation up to several nanoseconds. Using an electro-optical modulator, we investigate the thermal response of a W tip/Cu(111) surface from the low up to the high frequency regime. In combination with the raster-scanned laser focus, we have access to both time and spatially thermal response of the tip under optical excitation. [1] Weiss et al. APL. 63, 18 (1993) [2] Grafstrbm et al. J. of Vac. Sci. & Tech. B 9, 568 (1991) [3] Kloth et al. Rev. Sci. Instr. 87, (2016).

O 72.11 Wed 17:45 Poster B2

Microsecond Heat Pulses to Induce Phase Changes by Thermal Scanning Probe Lithography — •Samuel Zimmermann and Jürgen Brugger — Microsystems Laboratory, EPFL, Switzerland

Thermal scanning probe lithography (t-SPL) is an advanced lithography technique to create nanoscale surface structures by means of a heated atomic force microscopy tip. We use the fast heating and cooling rates accessible by t-SPL (~10^8 K/s) to locally induce phase changes in two organic materials, which are not attainable at the macroscale.

The first material is a fluorescent supramolecular polymer, which exhibits thermoresponsive luminescent behavior with two distinct fluorescence colors due to reversible aggregation of excimer forming moieties. Fast heating and cooling of small volumes on the order of attoliter with the thermal probe permits to quench the green fluorescent high-temperature state and to fabricate nanoscale structures with a fluorescence contrast below the optical diffraction limit.

The second material is silk fibroin, a protein extracted from the cocoons of the *Bombyx mori* moth, which exhibits a polymorphic structure with a difference in water solubility depending on its molecular arrangement. Applying microsecond heat pulses with a heated probe locally renders the material water-soluble by melting β-sheet crystallites, which act as crosslinks between the fibroin stands. Nanoscale patterns were fabricated with the heated probe, the contrast formation mechanism analyzed and a dry-etching transfer is demonstrated.

O 72.12 Wed 17:45 Poster B2

homemade nv-based scanning probe microscopy — •Ke Bian — College of Physics, Peking University, China

NV center host in diamond crystal is suitable for magnetic detection at nanoscale because of its high magnetic sensitivity and atomic size. We established a NV-based scanning probe microscopy (NVSPM) system aiming for scanning magnetometry and nanoscale nuclear magnetic resonance (NMR). Our home-built Pan-type scanner is rigid against both acoustic and electronic noise from ambient environment. We can obtain atomic resolution in STM mode and nanometer resolution in AFM mode. The high NA objective, microwave coplanar waveguide and kilo-gauss vector magnetic field are integrated inside the scanner. We also established confocal imaging and pulse sequence system for addressing single NV and coherent manipulation. By dynamical decoupling technique we can easily detect internal C13 nuclear spins with shallow NVs. The stable and accurate positioning ability paves the way for direct imaging of nanoscale magnetic particles or nuclear spin clusters on diamond surface.

O 73: Overview Talk: Christopher Lutz (joint session O/MA)

Time: Thursday 9:30–10:15 Location: H15

Invited Talk O 73.1 Thu 9:30 H15

Magnetic sensing by single-atom spin resonance in an STM — •Christopher Lutz — IBM Almaden Research Center, San Jose California, USA

Electron spin resonance (ESR) is widely used to obtain high energy resolution of magnetic properties in bulk samples. We use a low-temperature STM to perform ESR of individual magnetic atoms on a surface, and employ these atoms as atomic-scale magnetic sensors. This technique combines the high energy resolution of spin resonance with the single-atom control of STM. We drive spin resonance by using the large electric field available in the tunnel junction, and sense the spin by means of magnetoresistance, using a spin-polarized STM tip. Magnetic coupling between two iron atoms placed a few nanometers apart shows inverse-cube dependence on distance, which indicates dipole-dipole interaction. This yields a precise measure of the magnetic moment, which is then used to probe other atoms, such as the magnetic bits formed by individual holmium atoms. The STM can also drive spin resonance of titanium and copper atoms, which show free spin-1/2 behavior, in contrast to the large moment and easy-axis anisotropy of iron. Assembled arrays of low-spin atoms show exchange coupling that results in highly entangled magnetic states. Some isotopes exhibit hyperfine coupling, the interaction between the nucleus and the electrons of an atom, and the ESR spectrum reveals properties of the nucleus and the influence of the local atomic environment. The combination of STM with ESR thus provides a flexible tool for exploring nano-scale magnetism.

O 74: Focus Session: Growth, Properties and Application of Epitaxial Graphene (joint session DS/O/HL)

Graphene is the only 2D material, which up to now can be grown almost defect-free on large scales. The application of epitaxial concepts has turned out as a breakthrough in graphene research, because it provides control over the interface and surface structure of epitaxial graphene (EG) layers with atom-scale precision and in an efficient and technologically compatible way. A wide variety of physical phenomena have been observed in graphene-based structures, including topologically protected states, high charge carrier mobility, electron correlation or superconductivity. This versatility makes EG an ideal platform for the integration of graphene-based structures into electronic applications.

This Focus Session aims at fostering the cooperation between groups working in the field of the synthesis, characterization and integration of systems based on large, structurally well-ordered graphene layers. For this purpose it collects state-of-the-art contributions to all involved aspects of EG research, from the growth, functionalization and characterization to the integration of EG-based materials.

Organizers:

- Sibylle Gemming, Institut für Physik, TU Chemnitz, D-09107 Chemnitz
- Christoph Tegenkamp, Institut für Physik, TU Chemnitz, D-09107 Chemnitz

Time: Thursday 9:30–12:45 Location: H32

Invited Talk O 74.1 Thu 9:30 H32

Epitaxial graphene on SiC(0001) studied by electron spectroscopy and microscopy — •Florian Speck — Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany

The growth of epitaxial graphene (EG) on silicon carbide (SiC) by sublimation of silicon in an inert atmosphere has received considerable attention due to its scalability up to wafer size, and over the past years, the homogeneity of the graphene films could be significantly enhanced by a polymer assisted growth process [1]. Intricate transfer procedures can be dispensed with when semi-insulating SiC substrates are used, facilitating the use of EG in electronics. Yet, interfaces to other materials and the presence of a substrate can affect the graphene layers, e.g. with respect to their structural and electronic properties. As will be shown in this talk, EG grown on SiC(0001) constitutes an intriguing model system to study such interactions due to diverse possibilities of manipulating its properties for instance by intercalation of different elements at the interface to the substrate. To this end, we employ mainly surface science methods such as electron spectroscopies, low-energy electron diffraction and microscopy. Discussed topics include doping of EG induced by hexagonal SiC polytypes, interface modification by means of intercalation, dislocations in EG and investigations of graphene prepared by polymer assisted growth.

[1] M. Kruskopf et al., 2D Mater. **3**, 041002 (2016).

O 74.2 Thu 10:00 H32

Uniform large-scale quasi-freestanding monolayer and bilayer graphene on SiC — Davood Momeni Pakdehi[1], •Klaus Pierz[1], Stefan Wundrack[1], Johannes Aprojanz[2], T.T. Nhung Nguyen[3], Thorsten Dziomba[1], Frank Hohls[1], Andrey Bakin[4,5], Rainer Stosch[1], Christoph Tegenkamp[2,3], Franz J Ahlers[1], and Hans. W. Schumacher[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig — [2]Institut für Festkörperphysik, LU Hannover, Appelstraße 2, 30167 Hannover — [3]Institut für Physik, TU Chemnitz, Reichenhainer Straße 70, 09126 Chemnitz — [4]Institut für Halbleitertechnik, TU Braunschweig, 38106 Braunschweig, — [5]Laboratory of Emerging Nanometrology, TU Braunschweig, 38106 Braunschweig

Epitaxial graphene growth is often accompanied by step bunching of the underlying SiC substrate and graphene bilayer formation which can deteriorate the quality of graphene-based devices, e.g., the resistance quantization of the quantum Hall effect. We show AFM, STM, Raman and electronic transport data which indicate that improved buffer layer growth is the key to obtain homogenous large-area monolayer graphene. Particularly, the substantial impact of the so-far less regarded Ar flow rate on the graphene quality is investigated in this study and explained by a quasi-equilibrium model at the growing surface. The quality of our ultra-smooth graphene layers is proven by the high uniformity of quasi-freestanding graphene sheets obtained by hydrogen intercalation which is underlined by the very small resistance anisotropy of such samples on um and mm scales.

O 74.3 Thu 10:15 H32

Influence of minivalleys and Berry curvature on electrostatically induced nanostructures in gapped bilayer graphene — •Angelika Knothe and Vladimir Fal'ko — National Graphene Institute, University of Manchester, United Kingdom

We theoretically investigate the properties electrostatically confined nanostructures in gapped bilayer graphene (BLG). We show how the spectrum of subbands in a quantum wire in gapped BLG, and the energy levels in a quantum dot, manifest the minivalley structure and Berry curvature via the associated magnetic moment of the states in the low-energy bands. These features determine the degeneracies of the low-energy minibands / -levels and their valley splitting, which develops linearly in a weak magnetic field. In a quantum point contact, magneto-conductance reflects such degeneracies in the heights of the first conductance steps which develop upon the increase of the channel doping: $8e^2/h$ steps in a wide channel in BLG with a large gap, $4e^2/h$ steps in narrow channels, all splitting into a staircase of $2e^2/h$ steps upon lifting valley degeneracy by a magnetic field B. For quantum dots, we investigate how optical selection rules are influenced by the minivalleys and the orbital magnetic moment, as well as by shapes of the confinement.

References: A. Knothe and V. Fal'ko, Phys. Rev. B 98, 155435 (2018); H. Overweg, A. Knothe, V. I. Fal'ko, K. Ensslin, T. Ihn, et al., arXiv:1809.01920; R. Kraft, I.V. Krainov, V. Gall, A.P. Dmitriev, R. Krupke, I.V. Gornyi, R. Danneau, arXiv:1809.02458

O 74.4 Thu 10:30 H32

Tuning the doping level of graphene near the Van Hove singularity via ytterbium intercalation — •Hrag Karakachian, Philipp Rosenzweig, Stefan Link, Kathrin Müller, and Ulrich Starke — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

At extremely high doping levels, when pushing the Fermi level to the vicinity of graphene's Van Hove singularity (VHs), exotic electronic ground states are expected to occur driven by many-body interactions. These competing electronic phases such as chiral superconductivity, charge or spin density waves, find their stability based on the amount of doping induced in the graphene layer [1]. In this work, we present a method for effectively tuning graphene's doping level near its VHs. Epitaxially grown graphene on SiC(0001) is decoupled from the SiC substrate and strongly *n*-doped up to its VHs via ytterbium intercalation. By annealing the graphene/Yb system at different temperatures, a topological transition at the Fermi level is observed and a continuous shift in Dirac point energy is measured, indicating a change in carrier density. The Yb atoms go through different order patterns at different heating stages, and their concentration is modified as a function of temperature. These variations significantly affect the amount of charge transferred to the graphene layer and allow the systematic control of graphene's doping level near its VHs. Thus, the Yb intercalation technique can provide a reliable way of accessing and switching between different possible ordered electronic ground states in graphene.

[1] A.M. Black-Schaffer et al., J. Phys. CM **26**, 423201 (2014).

O 74.5 Thu 10:45 H32

Substrate induced nanoscale resistance variation in epitaxial graphene — •Anna Sinterhauf[1], Georg A. Traeger[1], Davood Momeni Pakdehi[2], Philip Schädlich[3], Florian Speck[3], Philip Willke[4,5], Thomas Seyller[3], Christoph Tegenkamp[3], Klaus Pierz[2], Hans Werner Schumacher[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [3]Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany — [4]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [5]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea

Electron transport in graphene is often crucially influenced by the underlying substrate which induces scattering mechanisms on a local scale. Using scanning tunneling potentiometry we investigate the transport properties of graphene on 6H-silicon carbide (0001) grown by polymer-assisted sublimation growth (PASG) down to the nanometer scale. We find a significant variation in the sheet resistance of up to 195% on neighboring terraces directly related to the stacking of the 6H-SiC substrate. Thus, our data clearly shows the strong influence of the substrate below the graphene layer on its local transport properties. In addition, we performed temperature dependent measurements to gain insight into the dominant scattering mechanism. This work is financially supported by the DFG through the SFB1073.

15 min. break.

Invited Talk O 74.6 Thu 11:15 H32

Patternable non-polar epigraphene for nanoelectronics and Dirac point physics — Vladimir Prudkovskiy[1,3], Yiran Hu[1], Hue Hu[1], Lei Ma[2], Claire Berger[1,3], and •Walt de Heer[1,2] — [1]Georgia Institute of Technology, Atlanta USA — [2]TICNN, Tianjin China — [3]Neel Institute, CNRS, Grenoble, France

Recently reported measurements of epitaxial graphene nanoribbons grown on sidewalls etched in the 0001 face of h-SiC, Nature,506, 349, (2014) indicate that both spin and valley degeneracies are lifted, resulting in the observed 10 micron scale, temperature independent, single channel transport. These highly unusual properties were further investigated in SiC wavers that were cut at an angle to the 0001 face were prepared at the Tianjin International Center for Nanoparticles and Nanostructures. The wafers were graphitized and 10 micron scale top gated Hall bar structures were patterned using standard lithography methods. Magnetotransport measurements revealed striking transport properties. Single channel ballistic transport is observed even at the Dirac point. Moreover, an anomalous quantum Hall plateau is observed. Its anomalous value is caused by a quantized current that does not have a Hall effect, and that is in parallel with an equal current that does have a Hall effect. These properties are likely to be caused by edge currents, with energies that are pinned at the Dirac point. The ballistic transport is essentially temperature independent and consistent with that observed in sidewall ribbons. These results indicate that nonpolar epigraphene is a promising candidate for epigraphene nanoelectonics and important for Dirac point physics.

O 74.7 Thu 11:45 H32

Epitaxial growth of ferromagnetic semiconducting $CrBr_3$ monolayer — •Weijiong Chen[1], Zeyuan Sun[1], Lehua Gu[1], Shiwei Wu[1,2], and Chunlei Gao[1,2] — [1]State Key Laboratory of Surface Physics, Key Laboratory of Micro and Nano Photonic Structures (MOE), Department of Physics, and Institute for Nanoelectronic Devices and Quantum Computing, Fudan University, Shanghai 200433, China — [2]Collaborative Innovation Center of Advanced Microstructures, Nanjing 210093, China

Recent discovery of two-dimensional (2D) ferromagnetic semiconducting materials greatly expands the family of 2D materials and invokes tremendous interests in novel magnetic related applications in 2D limit. Similar to most 2D materials, ferromagnetic 2D semiconductor is also firstly found in the mechanically exfoliated micrometer sized flakes, which hinders its further application. Here, we report the successful growth of ferromagnetic semiconducting monolayer $CrBr_3$ by compound source molecular beam epitaxy (CS-MBE). $CrBr_3$ compounds are directly evaporated onto the Highly Oriented Pyrolytic Graphite (HOPG) substrate and form $CrBr_3$ thin films with a precise thickness control. The atomic, electronic and magnetic properties were characterized by in-situ spin-polarized scanning tunneling microscopy. This growth method can be applied to other layered transition metal trihalides (LTMTs) as well, which provides a simple way of growing LTMTs for exploring their electronic and magnetic properties to the monolayer limit.

O 74.8 Thu 12:00 H32

Tuning the electronic properties of PbPb molecules by epitaxial graphene — •T.T.Nhung Nguyen[1], U. Gerstmann[2], T.N.Ha Nguyen[1], and C. Tegenkamp[1,3] — [1]TU Chemnitz, Germany — [2]Universität Paderborn, Germany — [3]Leibniz Universität Hannover, Germany

Functionalization of graphene aimed for its application in nanoelectronics is an important step. Among a variety of surface tailoring methods, molecular self-assembly gives rise to precisely control their interface by choosing appropriate molecules, e.g. non-planar leadphthalocyanine (PbPc). By means of scanning tunneling microscopy and density functional theory (DFT) we studied in detail the adsorption of PbPc on graphene/SiC(0001). Thereby, we used as template both n-doped monolayer (MLG) and neutral quasi-free monolayer graphene (QFML). On both surfaces PbPc forms almost identical monolayer structures, in agreement with DFT. Upon adsorption of the molecules, where the central atom points away from the surface, the benzene rings undergo pronounced distortions, where adjacent rings rotate and bend in opposite directions giving rise to a chiral single domain structure. Despite the same adsorption geometry, the molecular states of PbPc on these two surfaces are strongly shifted with respect to each other. First DFT results show that the negatively charged MLG is responsible for this effect.

Invited Talk O 74.9 Thu 12:15 H32

Intrinsic stacking domains in graphene on silicon carbide: A pathway for intercalation — Tobias A de Jong[1], Eugene E Krasovskii[2], Christian Ott[3], Rudolf M Tromp[4,1], Sense Jan van der Molen[1], and •Johannes Jobst[1] — [1]Leiden Institute of Physics, Leiden, The Netherlands — [2]Universidad del Pais Vasco, San Sebastián/Donostia, Spain — [3]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Erlangen, Germany — [4]IBM T. J. Watson Research Center, Yorktown Heights, USA

Graphene on silicon carbide (SiC) bears great potential for future graphene electronic applications because it is available on the wafer scale and its properties can be custom tailored by inserting various atoms into the graphene/SiC interface. It remains unclear, however, how atoms can cross the impermeable graphene layer during this widely used intercalation process. Here we demonstrate that in contrast to the current consensus, graphene layers grown in argon atmosphere on SiC are not homogeneous, but instead are composed of domains of different crystallographic stacking as they have been observed in other systems. We show that these domains are the AB and AC versions of Bernal stacking, that they are intrinsically formed during growth and that dislocations between domains dominate the (de)intercalation dynamics of hydrogen. Tailoring the resulting dislocation networks, e.g., through substrate engineering, will increase the control over the intercalation process and could open a playground for topological and correlated electron phenomena on the wafer scale.

O 75: Fundamentals of Catalysis I

Time: Thursday 10:30–13:00 Location: H5

O 75.1 Thu 10:30 H5

Coordination Effects in Model Rh1/Fe3O4 and Ir1/Fe3O4 Singe-Atom Catalysts — •Gareth Parkinson[1], Jan Hulva[1], Zdenek Jakub[1], Matthias Meier[1,2], Roland Bliem[1], Cesare Franchini[1,2], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]University of Vienna, Vienna, Austria

The coordination of the active site is thought to play a significant role in single atom catalysis, but precisely determining the local structure on high-area catalysts is extremely difficult. In this talk, I will report scanning probe microscopy, x-ray photoelectron spectroscopy (XPS) and temperature programmed desorption (TPD) results on the structure of Ir1/Fe3O4(001) and Rh1/Fe3O4(001) model single atom catalysts, and show that the coordination has dramatic consequences on CO adsorption. As prepared at room temperature, adatoms are twofold coordinated to surface oxygen, and hold on to CO until 650 K. Annealing the catalyst to successively higher temperatures results in five- and six-fold coordinated species, which adsorb CO even progressively more weakly. These results show that control of the local coordination environment is critical to design so-called single-atom catalysts, and that incorporation into the support can be as critical a deactivation mechanism for single atom catalysts as thermal sintering.

O 75.2 Thu 10:45 H5

CO-assisted stabilisation of single-atom Pt on ceria — •Nathan Daelman, Marçal Capdevila-Cortada, and Núria López — Institute of Chemical Research of Catalonia, Tarragona, Spain

Single-atom Pt on ceria has been proposed as a potential car exhaust catalyst that can achieve the DOE <150° challenge set forth by the EU.[1] Our work focuses on the system's applications in CO oxidation. The relevance of this reaction is far-reaching, since it is widely employed for single-atom detection. Nonetheless, its reactivity compared to nanoparticles is still under debate.[2,3]

We have identified a novel anchoring site for dispersed Pt atoms which yields a meta-stable catalyst on the oxygen-terminated (100) surfaces. Carbon monoxide stabilizes the single-atom site upon adsorption. Under oxygen-rich conditions O_2 then integrates into the lattice. From there on, the system converts through a percarbonate transition state to CO_2 gas. One oxygen anion remains in the lattice, effectively reducing the surface.

We acknowledge funding from the Spanish Ministry of Economy, Industry and Competitivity (ref.num.: CTQ2015-68770-R). We also wish to thank ICIQ, MareNostrum and BIFI for supplying us with access to their computing facilities.

[1] Betz, B., Müller, E., et al., 3rd Fundamentals and applications of Cerium Dioxide in catalysis, 2018, OP-2.1.

[2] Jones, J., Xiong, H., et al., Science, 2016, 353, 150-154.

[3] Ding, K., Gulec, A., et al., Science, 2015, 350, 189-192.

Invited Talk O 75.3 Thu 11:00 H5

Structure evolution of oxide-supported metal nanoparticles under different conditions — •Yuemin Wang — Institute of Functional Interfaces, Karlsruhe Institute of Technology, Germany

A fundamental understanding of nanostructured metal oxides and oxide-supported metal nanoparticles (NPs) is among the most important and challenging topics in catalysis and nanoscience. Here, we present our recent work on various metal/oxide NPs (Cu/CeO_2, Pt/CeO_2 and Pt/Al_2O_3). The study combining in-situ IR spectroscopy (polarization-resolved IRRAS on model systems and IR transmission on powders), high-resolution TEM and DFT calculations allowed us to gain deep insight into structural, electronic and reactive properties of the metal/oxide systems under different conditions. The results revealed that the atomic structure of pristine and metal-decorated oxide surfaces can vary substantially depending on activation or reaction conditions. For Cu/CeO_2, we will discuss the atomic structure of ultrafine copper clusters (bilayer, 1.0-1.5 nm) and the dynamic behavior under reactive gases at elevated temperatures. For Pt/CeO_2 and Pt/Al_2O_3 systems, we will focus on the structure evolution of various Pt clusters during the course of activation or reaction.

O 75.4 Thu 11:30 H5

Observing diffusion and morphology changes of small metal clusters via scanning tunneling microscopy — •Barbara A J Lechner, Ke Zhang, Alexander Bourgund, Fabian Knoller, Ueli Heiz, and Friedrich Esch — Department of Chemistry & Catalysis Research Center, Technical University of Munich, Lichtenbergstr. 4, D-85748 Garching

Metal clusters are partway between molecular and bulk systems and thus exhibit special physical and chemical properties: Atoms can rearrange within a cluster to form different structural isomers, clusters of different size can exhibit a different diffusivity across the same support. Here, we show how scanning tunneling microscopy (STM) can be used to investigate such dynamical behavior of individual clusters. By operating our STM with a specially developed FastSTM add-on module, we followed steady state diffusion of Pd_n $(1 \leq n \leq 19)$ clusters and atoms inside the pore of a hexagonal boron nitride nanomesh on Rh(111). While atoms diffuse along the rim of a pore, a small cluster experiences a corrugation in the potential energy landscape and jumps between six sites around the center of the pore. Furthermore, we observed reversible cluster isomerization in situ. In another example, we observed an irreversible decrease in apparent height of Pt_n clusters supported on an $Fe_3O_4(001)$ single crystal surface with increasing temperature. Such a morphological change without concomitant changes in cluster coverage suggests that the cluster-support interface changes with temperature, possibly favoring flattened clusters over spherical ones.

O 75.5 Thu 11:45 H5

Modelling Ostwald ripening beyond mean-field models — •Elisabeth M. Dietze and Philipp N. Plessow — Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology, Karlsruhe, Germany

Transport of atoms and molecules via the gas-phase plays an important role in many processes in heterogeneous catalysis. One of the challenges for heterogeneous catalysts in industry is deactivation due to sintering. For example, platinum particles are widely used in exhaust gas after treatment, but suffer from sintering trough ripening by volatile PtO_2 under oxidizing conditions.

We have recently proposed a kinetic Monte Carlo (kMC) model for the explicit simulation of gas-phase mass transport.[1] On small length scales that correspond to typical distances between nanoparticles, transport in model systems was found to deviate significantly from Fick's laws. We are currently exploring, how that affects sintering, when compared with mean-field models suggested in the literature. [2-3]

References: [1] Dietze, E. M.; Plessow, P. N., J. Phys. Chem. C 2018, 122 (21), 11524-11531. [2] Campbell, C. T.; Mao, Z., ACS Catal. 2017, 7 (12), 8460-8466. [3] Plessow, P. N.; Abild-Pedersen, F., ACS Catal. 2016, 6 (10), 7098-7108.

O 75.6 Thu 12:00 H5

Ru/TiO_2 catalysts in the CO methanation: influence of the TiO_2 morphology on the activation and the chemical nature of Ru investigated by operando X-ray absorption spectroscopy — Shilong Chen[1], •Joachim Bansmann[1], Ali Abdel-Mageed[1], Dan Li[2], Weixin Huang[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Dept. of Chemical Physics, University of Science and Technology of China, Hefei, China

The selective CO methanation recently proved to be a competitive substitute for the preferential CO oxidation in the purification of CO_2-rich H_2 feed gases. In this contribution, we concentrate on the physical and chemical properties of Ru nanoparticles on Ru/TiO_2 catalysts in the CO methanation using TiO_2 supports with different morphologies. The catalysts were investigated at the ID 24 beamline at the ESRF (Grenoble) using operando X-ray absorption spectroscopy (XAS) at the Ru K edge in an idealized reformate at atmospheric pressure (0.6% CO, 3% N_2, balance H_2) at 190°C. Ru/TiO_2-{001} catalysts experience a much faster activation, however, also a more pronounced deactivation compared to Ru/TiO_2-{100} catalysts. Measurements in the XANES region showed a higher content of oxidic species on Ru/TiO_2-{100} catalysts during the activation period which seems to be related to the lower activity. These findings will be discussed with respect to simultaneously recorded IR data and results obtained from different Ru/TiO_2 catalysts used in our group.

O 75.7 Thu 12:15 H5

Density functional study of hydrogen adsorption on 55-atom Pt-Ni nanoclusters — •Olli Ahlstedt[1] and Jaakko Akola[1,2] — [1]Laboratory of Physics, Tampere University of Technology, Finland — [2]Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway

Density functional theory calculations were performed on small 55-atom Pt-Ni nanoclusters to study their activity towards the hydrogen evolution reaction (HER). Two Pt_nNi_{55-n} compositions, $Pt_{12}Ni_{43}$ and $Pt_{20}Ni_{35}$, were studied in the gas phase and on an Al_2O_3 support. The critical hydrogen coverages were determined using the method based on the differential free energy of hydrogen adsorption. The free energy of hydrogen adsorption, ΔG^*_H, was used as a descriptor of the HER activity.

Ni_3 hollow sites were discovered to be the strongly binding sites for hydrogen. The clusters adsorb approximately four H atoms per facet before the hydrogen adsorption becomes endergonic, therefore the critical hydrogen coverages on the clusters are high. The obtained ΔG^*_H descriptor values are smaller than 0.1 eV in the gas phase and on the support, suggesting that the clusters are catalytically active towards HER.

O 75.8 Thu 12:30 H5

Bimetallic PdPt Alloy Nanocluster Arrays on Graphene/Rh(111): Formation, Stability, and Dynamics — •Fabian Düll, Udo Bauer, Florian Späth, Philipp Bachmann, Johann Steinhauer, Hans-Peter Steinrück, and Christian Papp — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander- Universität Erlangen-Nürnberg, Germany

Alloy catalysts often have superior properties compared to their single metal counterparts. We studied bimetallic PdPt alloy nanocluster arrays supported on a chemically inert graphene/Rh(111) Moiré. The clusters are well-ordered, separated, and have a small size distribution; thus, they are an intriguing model system for catalysis bridging the materials gap by introducing various facet and edge sites. Using in situ high-resolution XPS, we followed the site occupation and dynamic changes of the metal distribution during CO adsorption and thermal treatment [PCCP, 2018, 20, 21294]. Annealing of the as-prepared nanoclusters after exposure to CO to 550 K leads to a restructuring towards a more 3D shape and to a replacement of Pt atoms at the cluster edges by Pd. The facets are dominated by Pt. Additionally, the nanoclusters are stabilized, as repeated CO adsorption and desorption cycles cause no further changes. Interestingly, we observe dynamical changes during heating or when applying a CO- or O2-stream at constant temperatures: CO molecules rearrange from terrace to edge sites, and Pt atoms move back to the particle edges. These effects are only found at elevated temperatures in the presence of CO and disappear when the system cools down in a vacuum.

O 75.9 Thu 12:45 H5

Coverage and temperature dependent size and distribution variations of entrapped Pt-nanoclusters on h-BN/Rh(111) — •Manuel Meusel, Fabian Düll, Simon Schötz, Florian Späth, Udo Bauer, Philipp Bachmann, Johan Steinhauer, Hans-Peter Steinrück, Andreas Bayer, and Christian Papp — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

UHV methods provide a powerful tool to investigate surfaces down to the atomic level. However, a large material gap exists between highly defined single crystalline surfaces under UHV conditions and real life materials. One route to bridge this material gap are, at first, more complex surfaces with steps, followed by nanoclusters with mainly edges and corners. By using the Moiré pattern of hexagonal boron-nitride (h-BN) on Rh(111), it is possible to prepare highly defined arrays of separated metal nanoclusters. These systems are promising candidates as model systems for the complex surfaces of heterogeneous catalysts, while still being accessible to investigations via surface science methods. Therefore, the controlled fabrication and understanding of such systems is crucial. We conducted STM and XPS investigations on the coverage- and temperature-dependence of distribution and size of the Pt nanoclusters in the h BN/Rh(111) nanomesh at sub-monolayer coverages. Above 0.1 ML of Pt, we observe well-ordered nanoclusters with a uniform shape. Below this coverage, an inhomogeneous appearance suggests the presence of smaller, more mobile clusters. Further, we discuss the temperature-dependent sintering behaviour.

O 76: Plasmonics & Nanooptics V: Nanostructures and Nanoantennae

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

O 76.1 Thu 10:30 H8

Near-field characterization of V-shaped plasmonic antennas — •Lukas Naumann, Mike Prämassing, and Stefan Linden — Physikalisches Institut der Universität Bonn, D-53115 Bonn

Optical metasurfaces offer fascinating possibilities for controlling light e.g. beam-shaping, steering or polarizing conversion [1,2]. The functionality of a metasurface is governed by the geometry of its subwavelength building blocks, so called metaatoms. One possible type of a metaatom is a V-shaped plasmonic antenna, providing two plasmonic resonances which are tunable by the geometric parameters and can introduce arbitrary phase shifts to the scattered light [2].

Here we investigate the near-field distribution of single V-shaped antennas by the means of scattering-type scanning near-field optical microscopy (s-SNOM) in transmission mode configuration with an interferometric detection scheme, enabling amplitude- and phase-resolved measurements. Depending on wavelength and polarisation of the incoming laser beam as well as on the size of the antennas either the fundamental (asymmetric) mode, the first higher (symmetric) mode or a mixture of both can be excited. The relative phase offsets between different antennas can be deduced from our measurements and can be explained by simple theoretical considerations.

[1] Flat optics with designer metasurface; Nanfang Yu, Federico Capasso; Nature Naterials 13, 139-150 (2014)

[2] Light Propagation with Phase Discontinuities: Generalized Laws of Reflection and Refraction; Federico Capasso et al.; Science 334 (6054), 333-337 (2011)

O 76.2 Thu 10:45 H8

Fabrication of Plasmonic Nanostructures by He$^+$ and Ga$^+$ Milling — •Michael Westphal[1], Sven Stephan[2], Vladimir Smirnov[2], Daniel Emmrich[1], Henning Vieker[1], Andre Beyer[1], Martin Silies[2], and Armin Gölzhäuser[1] — [1]Bielefeld University, Germany — [2]Oldenburg University, Germany

Plasmonic nanostructures are essential for controlling and directing light on the nanoscale. While fabrication techniques like standard electron beam lithography (EBL) methods or focused ion beam (FIB) milling with Ga$^+$ ions are approaching their limit in the 10-nm-regime, ion beam milling with He$^+$ ions is capable of milling features below 6 nm [1]. We will show a combined approach using a Ga$^+$ FIB for milling large features and employing the fine resolution of the helium ion microscope (HIM) for milling small features. We will discuss different patterning strategies to optimize the writing speed and minimize substrate swelling. In addition, the problem of quantifying the sizes of milled gaps will be addressed and an automated, reproducible approach for measuring the size of written features will be demonstrated.

[1] H. Kollmann et al., Nano Letters. 14, 4778-4784 (2014).

O 76.3 Thu 11:00 H8

A freestanding 40 nm thick metasurface lens — •Till Leuteritz, Mike Prämassing, and Stefan Linden — Physikalisches Institut, Universität Bonn, D-53115

Miniaturization of electronics has lead to a rapid rise of new technologies like cellphones and tablets. The limiting factor of a cellphones thickness today is the lens. A solution to reduce the thickness of lenses was presented by A. Francesco et al in 2012 [1]. They demonstrated a metasurface consisting of V-shaped antennas which introduces the phase profile required for lensing. Even though most metasurfaces are a few ten nanometers thick they are typically fabricated on a 100 um thick inflexible glass substrate. In our work we present a solution to overcome this problem.

Considering Babinets principle, we use an inverted design of V-shaped plasmonic slot antennas in a freestanding 40nm gold film. They are produced by milling the V-shaped structures into carbon film with a focused ion beam. Thermal evaporation of the gold film followed by a plasma etching step to remove the carbon yields the desired structure.

We find an agreement between modes of an individual V-shaped antenna determined by energy electron loss spectroscopy and simulations done with a finite elemente solver. In addition we experimentally show the focusing of our metasurface lens and the simulations to optimize it.

[1] Aieta, Francesco, et al., Nano letters 12.9 (2012): 4932-4936.

O 76.4 Thu 11:15 H8

Plasmonic resonators in 1D and 2D: quality factor of resonances and near-fields — •Manuel Gonçalves[1], Gregor Neusser[2], Christine Kranz[2], and Othmar Marti[1] — [1]Ulm University - Institute of Experimental Physics, Ulm, Germany — [2]Ulm University - Institute of Analytical and Bioanalytical Chemistry, Ulm, Germany

Plasmonic particles present broad optical reasonances and reach therefore only small Q-factors. In many applications where narrow resonances are required 1-dimensional multilayered metal-dielectric films and periodically arranged 2-dimensional nanostructures can form resonators performing much better than single particles. The design of theses resonators can be optimized for reflectance and/or transmittance sensing applications, or for large near-field enhancement. We show how 1D multilayered metal-dielectric thin films with quality factors over 100 can be fabricated. We also have fabricated 2D nanostructures based on deep grooves milled in crystalline metal films, which achieve large Q-factors, strongly confine light at the grooves and simultaneously present remarkable dependence of the reflectance on the polarization of the incident light. We present experimental results as well as simulations.

O 76.5 Thu 11:30 H8

Ingenious 3D gap-plasmonic Ag@Ag strawberry galactic nanostructure for SERS detection — •Qun Fu[1,2], Huaping Zhao[1], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany — [2]Institute of Nanochemistry and Nanobiology, School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, China

The realization of the strongly confined and enhanced electromagnetic (EM) field with gap-plasmon resonance at ultrasmall (sub-10-nm) gaps is crucial for ultrasensitive SERS (surface-enhanced Raman scattering) detection. However, most traditional methods for creating gap-plasmon are based on the lithography techniques, and it remains a challenge to cost-effectively produce high-density sub-nanometer gaps over large-scale. An ingenious 3D gap-plasmonic Ag@Ag strawberry galactic nanostructure is therefore developed by employing an UTAM (ultrathin alumina mask) nano-patterning process. The UTAM-based nanopatterning strategy enables to fabricating Ag@Ag strawberry galactic nanostructures with multiple ultra-small SERS hotspots in super-high density and over large scale. A strongly enhanced Raman signal (detection limit of R6G molecule as low as 10-16 M) with good reproducibility is obtained based on Ag@Ag strawberry galactic nanostructures, attributing to the coupling effect at multiple hot spots around the six kinds of nanogaps and the intense EM fields at numerous ordered roughness and tips in two-level particle arrays of this structure.

O 76.6 Thu 11:45 H8

Near-field characterization of plasmonic slot waveguides in single-crystalline gold films — •Mike Prämassing[1], Hans-Joachim Schill[1], Matthias Liebtrau[1], Stephan Irsen[2], and Stefan Linden[1] — [1]Physikalisches Institut Universität Bonn, D-53115 — [2]Center of advanced european studies and research (caesar), Bonn, D-53175

Plasmonic slot waveguides (PSW's) consist of a sub-wavelength gap engraved in a thin metal film. PSW's support guided plasmonic modes with a lateral confinement siginificantly below the diffraction limit, while sustaining propagation over several microns. Therfore PSW's are attractive canditates e.g. as building blocks for integrated opto-electronic circuits [1], or for enhanced coupling to quantum emitters [2]. Here, we investigate the dependency of the the effective mode index n_{eff} and the propagation length L_{p} on the slot width. For the first time, we use focused ion beam milling on chemically grown 50 nm thick single-crystalline gold flakes to fabricate down to 50 nm wide PSW's. We utilize scattering-type scanning near-field optical microscopy (s-SNOM) in transmission mode configuration with an interferometric detection scheme for amplitude- and phase-resolved measurements. A 2D model-function is fitted to the measured near-field distributions in order to extract n_{eff} and L_{p}. Our experimental results are in accordance with finite element simulations. The presented results may offer design rules to optimize PSW's for potential future applications.

[1]Gramotnev, and Bozhevolnyi. Nature photonics 4, 83 (2010).

[2]Jun et al. Phys. Rev. B 78, 153111 (2008).

O 76.7 Thu 12:00 H8

Visible light operation of a single-crystalline silver plasmonic nanocircuit — •Christian Schörner, Subhasis Adhikari, and Markus Lippitz — University of Bayreuth, Germany

The miniaturization of optical devices is of great importance for future ultrafast integrated nano-optical circuitry. High quality plasmonic nanostructures, such as nano-antennas, nano-resonators and waveguides, need to be fabricated by focused-ion beam milling of single-crystalline metal flakes or films. However, for waveguide applications, gold limits the operation wavelength to the infrared spectral range. Here, we demonstrate multimode operation of a silver plasmonic two-wire transmission line in the visible range. We further remotely excite 20nm fluorescent beads along the waveguide and shift excitation centers by applying different superpositions of the available waveguide modes.

O 76.8 Thu 12:15 H8

Strong Spatial and Spectral Localization of Surface Plasmons in Individual Randomly Disordered Gold Nanosponges — •Anke Korte[1], Jinhui Zhong[1], Abbas Chimeh[1], Felix Schwarz[2], Juemin Yi[1], Dong Wang[3], Jinxin Zhan[1], Peter Schaaf[3], Erich Runge[2], and Christoph Lienau[1] — [1]Institut für Physik & Center of Interface Science, Carl von Ossietzky Universität, 26129 Oldenburg, Germany — [2]Institut für Physik & Institut für Mikro- und Nanotechnologien MacroNano, TU Ilmenau, 98693 Ilmenau, Germany — [3]Institut für Werkstofftechnik & Institut für Mikro- und Nanotechnologien MacroNano, TU Ilmenau, 98693 Ilmenau, Germany

Porous nanosponges, percolated with a three-dimensional network of 10 nm sized ligaments, recently emerged as promising substrates for plasmon-enhanced spectroscopy and (photo)catalysis. Experimental and theoretical work suggests surface plasmon localization in some hot-spot modes as the physical origin of their unusual optical properties, but so far the existence of such hot-spots has not been proven. Here we use scattering-type scanning near-field nanospectroscopy on individual gold nanosponges to reveal spatially and spectrally confined modes at 10 nm scale by recording local near-field scattering spectra. High quality factors of individual hot-spots of more than 40 are demonstrated, predicting high Purcell factors up to 10ˆ6. The observed field localization and enhancement make such nanosponges an appealing platform for a variety of applications ranging from nonlinear optics to strong-coupling physics.

O 76.9 Thu 12:30 H8

Electric, magnetic and electromagnetic hot spots — •Vlastimil Křápek, Michal Horák, Martin Hrtoň, Filip Ligmajer, and Tomáš Šikola — Central European Institute of Technology, Brno University of Technology, Purkyňova 123, 612 00 Brno, Czech Republic

We study plasmonic antennas featuring areas of extremely concentrated electric or magnetic field, known as hot spots. To this end we use optical spectroscopy and electron beam spectroscopy together with numerical modeling. We combine two types of electric-magnetic complementarity to increase the degree of freedom for the design of the antennas: bow-tie and diabolo duality and Babinet's principle. We evaluate the figures of merit for different plasmon-enhanced optical spectroscopy methods: field enhancement, decay rate enhancement, and quality factor of the plasmon resonances. The role of Babinet's principle in interchanging electric and magnetic field hot spots and its consequences for practical antenna design are discusses. Finally, we propose Babinet-type dimer antenna featuring electromagnetic hot spot with both the electric and magnetic field components treated on equal footing.

We particularly focus on antennas featuring magnetic hot spots in the THz spectral range, and discuss their application in plasmon-enhanced electron spin resonance.

O 76.10 Thu 12:45 H8

First-order perturbation theory for material changes in the surrounding of open optical resonators — •Steffen Both and Thomas Weiss — 4th Physics Institute and Research Center SCoPE, University of Stuttgart

Nanophotonic structures such as photonic crystals or plasmonic nanoparticles allow the realization of optical resonances with strong electromagnetic near-fields. In such structures, even tiny material changes in the environment can have significant influence on the resonances frequencies. This effect is the key to various kinds of optical sensing applications [1]. So far, the modeling of these interactions often relies on extensive numerical simulations, which can be rather inefficient, since in many practical cases, the variations in the material properties are extremely small. Here, we present a simple perturbation theory, that is particularly suited for these cases, and that allows to very efficiently calculate the resonance shifts and linewidth changes induced by small material modifications in the surrounding of almost any kind of open optical resonator. Our main result is a simple integral expression over the fields of the unperturbed system, which extends previous works from the field of resonant state expansion [1-4].

[1] T. Weiss, et al., Phys. Rev. B **96**, 045129 (2017).

[2] M. B. Doost, et al., Phys. Rev. A **90**, 013834 (2014).

[3] J. Yang, et al., Nano Lett. **15**, 3439 (2015).

[4] T. Weiss et al., Phys. Rev. B **98**, 085433 (2018).

O 77: Organic Molecules on Inorganic Substrates V: Solid-Liquid Interfaces, Self-Organization, Ordering

Time: Thursday 10:30–13:15 Location: H9

O 77.1 Thu 10:30 H9

Self-assembly of phospholipids on Au(111) as a model system for the cytoplasmic membrane — •Iris Dorner[1], Ulrike Diebold[1], Gerhard J Schütz[1], and Stijn F L Mertens[1,2] — [1]TU Vienna, Institute of Applied Physics, Wiedner Hauptstr. 8-10/134, 1040 Vienna, Austria — [2]Lancaster University, Department of Chemistry, LA1 4YB, Lancaster, United Kingdom

Lateral organization of lipids and proteins plays a crucial role in biological processes such as cell signalling. In order to understand the interactions governing the organization of amphiphilic molecules, a model system must provide access to nanoscale information at the interface between a 2D-confined phase and liquid water. We present such a model system in the self-assembled monolayer and bilayer of phospholipids on Au(111). We study the stages of adsorption and the dynamics of our model system with complementary imaging techniques, electrochemical scanning tunnelling microscopy, atomic force microscopy and single-molecule fluorescence microscopy. These shed light on the initial adsorption mechanism via the monolayer, bilayer formation, as well as the much discussed formation of ordered lipid domains such as rafts.

O 77.2 Thu 10:45 H9

Controlling the surface adsorption of polyoxometalates from the liquid phase — •Maria Glöss[1,2], Ricarda Pütt[1], Marco Moors[2], Emmanuel Kentzinger[2], Wim Pyckhout-Hintzen[2], and Kirill Monakhov[3] — [1]RWTH Aachen — [2]Forschungszentrum Jülich GmbH — [3]Leibniz-Institute of Surface Engineering

Vanadium containing polyoxometalates (POMs) offer a wide range of potential applications due to their structural diversity appealing electronic properties. The probability of switching between multiple redox states without structural changes of the molecular system is one of the significant prerequisites for the development of molecule-based data storage devices.

For a technical implementation of POMs it is crucial to elucidate their adsorption behaviour on conductive substrates. In this study we investigate the droplet deposition from the liquid phase in order to correlate the molecular arrangement of POMs in solution and on weakly bonding surfaces.

Therefore, we characterise the adsorption behaviour of a functionalised Wells-Dawson-type POM on HOPG via STM and XPS. For the characterisation of the liquid phase SAXS is used. Depending on the water amount in the POM solution a complex agglomeration mechanism of the molecules is observed, which strongly affects the surface appearance after deposition reaching from defect-rich 2D molecular layers up to the formation of isolated metal-oxo cluster arrangements.

O 77.3 Thu 11:00 H9

Conformation control of peptides on surfaces via metal coordination — •Sabine Abb[1], Elise Duquesne[2], Ludger Harnau[1], Stephan Rauschenbach[1,3], and Klaus Kern[1,4] — [1]Max Planck Institute for solid state research, Stuttgart, Germany — [2]CNRS Paris, France — [3]University of Oxford, UK — [4]Ecole Polytechnique Fédérale de Lausanne, Switzerland

The conformation of peptides is defined by its sequence of amino acids and generally depends on the environmental conditions such as pH, salt concentration or temperature. Additionally, the coordination to metal centers can change the conformation, inducing also a change in the functionality of the peptide. Nearly half of all peptides/proteins are associated with metal coordination.

In this work, the metal-coordination complex is deposited by ES-IBD and investigated by STM. Here, we present the tailored conformation control of angiotensin-II (8 amino acids) on Au(111) by coordination to different metal centers. This is the first step towards rational design of surface supported peptide coordination complexes that can be relevant for different applications such as biomimetic catalysis.

O 77.4 Thu 11:15 H9

Specific Interactions of Organic Solvents on Hydrophobic Surfaces — •Annemarie Pfnür[1], Johannes Will[2], Florian Bertram[3], Milena Lippmann[3], and Tobias Unruh[1] — [1]Institute of Crystallography and Structural Physics, Friedrich-Alexander-Universität Erlangen- Nürnberg (FAU), Staudtstr. 3, 91058 Erlangen, Germany — [2]Department of Materials Science and Engineering, Chair of Micro- and Nanostructure Research, Friedrich-Alexander-Universität Erlangen- Nürnberg (FAU), Cauerstr. 6, 91058 Erlangen, Germany — [3]DESY Photon Science, Notkestr. 85, 22607 Hamburg, Germany

The stabilization mechanism of organic nanoparticles in aqueous dispersion produced by liquid antisolvent precipitation without additional stabilizers is under discussion. It is assumed that the solvent used in the production process forms a stabilizing layer at the interface of the nanoparticles.

In order to study this stabilizing layer, we developed a well defined planar model system for the liquid/solid interface. In a liquid cell, the interface of the sample to various solvents and solvent-water mixtures was studied by in-situ X-ray reflectometry (XRR).

A comprehensive analysis with a uniform model for all measurement curves demonstrated the existence of a solvent layer, with a thickness increasing systematically with the solvent concentration of the solvent-water mixture. The layer formation is correlated to the molecular size, the molar volume, as well as the polar and the hydrogen bond fraction of the Hansen solubility parameters.

O 77.5 Thu 11:30 H9

Molar Ratio of Building Blocks in Controlling the Domain Size of an Imine-Covalent Organic Framework — •Vipin Mishra[1], Vivek K Yadav[2], Jayant K Singh[2], and Thiruvancheril G Gopakumar[1] — [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

Imine COF[1,2] (covalent organic framework) based on Schiff base reaction between p-phenylenediamine (PDA) and benzene-1,3,5-tricarboxaldehyde (TCA) is prepared on the HOPG-air interface. Using a combination of STM, AFM and XPS the microscopic formation of imine COF is confirmed. Role of the molar ratio of TCA and PDA has been explored and large smooth domains up to 2 um are formed for high TCA ratio (>2) compared to PDA. It is also observed that the quality of imine COF is strongly influenced by the presence of water atmosphere during the Schiff base reaction. The electronic property of imine COF is understood by experiment (tunneling spectroscopy) and dispersion corrected density functional theory (DFT) calculation. It is observed that the imine COF is semiconducting in nature with a band gap of ~1.9 eV. The calculation also indicates that the frontier orbitals are delocalized over the framework of imine COF. The calculated cohesive energy shows that the stability of imine COF is comparable to that of graphene.

[1] Y. Yu et al. Chem. Commun., 2016, 52, 8317. [2] X. Lirong et al. Angew. Chem. Int. Ed., 2014, 53, 9564.

O 77.6 Thu 11:45 H9

Structure of individual polythiophene molecules on Ag(111) — •Erik Schreck[1], Stefan Förster[1], and Wolf Widdra[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

This talk presents a low-temperature scanning tunneling microscopy (STM) study of Poly(3-hexylthiophene) (P3HT) polymers on Ag(111). Submonolayer films were prepared by electrospray deposition under ultra-high vacuum conditions. Side chain resolved STM images reveal individual polymers and polymers forming condensed 2D structures. The distributions of end-to-end distance, radius of gyration and persistence length are derived by image analysis and are interpreted in terms of a 2D self-avoiding random walk.

In 2D condensates, we find enlarged persistence length and distinct bending angles between parallel polymer segments in comparison to isolated polymers. For the individual chains, the persistence length is smaller on Ag(111) than for Au(001)[2], which is discussed based on modified polymer-substrate interactions.

[1] S. Förster and W. Widdra, J. Chem. Phys. 141, 054713 (2014)
[2] S. Förster, E. Kohl, M. Ivanov, J. Gross, W. Widdra and W. Janke, J. Chem. Phys. 141, 164701 (2014)

O 77.7 Thu 12:00 H9

Metalation and coordination reactions of 2H-meso-trans-di(p-cyanophenyl)porphyrin on Ag(111) with coadsorbed cobalt atoms — •Jan Kuliga, Liang Zhang, Michael Lepper, Hans-Peter Steinrück, and Hubertus Marbach — Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

The controlled fabrication of functional molecular nanoarchitectures on surfaces is in the focus of our research activities. Thereby, we follow a bottom-up approach in which we rely on the adsorption behavior, i.e., self-assembly and in situ reactions of porphyrin derivatives as prototype functional molecules. In this context, we investigated the metalation and coordination reactions of Co with 5,15-bis(para-cyanophenyl)-10,20-bisphenylporphyrin (2HtransDCNPP) on a Ag(111) surface by scanning tunneling microscopy. At room temperature, 2HtransDCNPPs self-assemble into a well-ordered supramolecular structure stabilized by van der Waals interactions and intermolecular hydrogen bonding. The metalation to CotransDCNPP can be realized by pre- or post-deposition of Co atoms onto the Ag(111) surface. Interestingly, with *excess* Co material we observe the formation of peculiar structures appearing as 3 to 7 protrusion motifs in STM, with the dominating motif the 5-protrusion appearance.[1] The motifs could be identified through bias-dependent STM as 2 to 6 CotransDCNPPs coordinated by central Co atoms through peripheral cyano groups.

[1] Kuliga, et al., PCCP 20 (2018) 25062

O 77.8 Thu 12:15 H9

Aurophilic interactions on surfaces — •Thorsten Wagner[1], Michael Brunthaler[1], Michael Györök[1], Petra Gründlinger[1], Uwe Monkowius[2], and Peter Zeppenfeld[1] — [1]Institute of Experimental Physics, Johannes Kepler University, Linz, Austria — [2]School of Education, Johannes Kepler University, Linz, Austria

Metallophilicity describes attractive interactions between two or more metal atoms with closed shell configurations (i.e. d^8, d^{10}). Metal complexes containing gold in the formal oxidation state +I exhibit a very strong interaction of this kind, which is often decisive for their arrangement in the solid state [1,2]. To study this aurophilic interaction on surfaces, we prepared by physical vapor deposition films with a thickness of just a few layers of 2-naphthyl-isonitrile-gold(I)-chloride on Au(111) and Au(110) surfaces. The deposition was monitored by differential reflectance spectroscopy (DRS) and photoelectron emission microscopy (PEEM). After growth, the structure was characterized by means of scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). In the case of the Au(111) substrate, we are able to confirm an anti-dimer structure similar to the bulk one demonstrating that the Au-Au interaction is preserved in the ultrathin films. For the Au(110) substrate, we did not observe the characteristic crossed swords arrangement [2]. In fact, the (1×2) reconstruction of the substrate surface is lifted upon adsorption of the molecules suggesting a sizable interaction between Au(I) complexes and Au substrate.

[1] P. Pyykkö, Chem. Rev. **97**, 597 (1997).
[2] E. Hobbollahi *et al.*, Inorg. Chem. Com. **65**, 24 (2016).

O 77.9 Thu 12:30 H9

Adsorption and Electronic Properties of N-Heteropolycyclic Molecules on Metal Surfaces — •Mohsen Ajdari[1], Friedrich Maass[1], Matthias Müller[2], Christoph Hendrich[2], Uwe H. F. Bunz[2], A. Stephen K. Hashmi[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg — [2]Organisch-Chemisches Institut, Universität Heidelberg

Small molecule organic semiconductors based on N-heteropolycyclic aromatic compounds are promising candidates for a variety of (opto) electronic applications. In these molecules, introduction of nitrogen in their aromatic backbone in its pyridine form decreases the energy of both HOMO and LUMO, resulting in an improved stability due to an increased ionization potential and electron affinity of organic semiconductor, while the optical gap remains almost constant.

Understanding the adsorption and electronic properties of these molecules on inorganic substrates provides important insights into the charge transfer properties at organic/inorganic interface. High resolution electron energy loss spectroscopy (HREELS) is a powerful tool for investigating both the adsorption geometry via vibrational excitations and electronic properties of the molecules by utilizing electrons with sufficient energy to excite electronic transitions. In this study, HREELS is used to determine the adsorption and electronic properties of a new class of N-heteropolycyclic molecules as a function of coverage on Au(111).

O 77.10 Thu 12:45 H9

Formation of Si/organic interfaces using alkyne-functionalized cyclooctynes — Christian Länger[1], •Julian Heep[1], Paul Nikodemiak[2], Tamam Bohamud[2], Patrick Kirsten[1], Ulrich Höfer[2], Ulrich Koert[2], and Michael Dürr[1] — [1]Justus-Liebig-Universität, 35392 Gießen — [2]Philipps-Universität, 35037 Marburg

Controlled organic functionalization of semiconductor surfaces requires chemoselective adsorption of bifunctional molecules on the surface. Here we show for ethynyl-cyclopropyl-cyclooctyne (ECCO), an alkyne-functionalized cyclooctyne, that such chemoselective adsorption can be achieved on Si(001) despite the high reactivity of both functional groups in the molecule, i.e., the strained triple bond of cyclooctyne and the terminal triple bond. XPS and STM results clearly indicate that ECCO adsorbs selectively on Si(001) via a [2+2] cycloaddition of the strained triple bond without reaction of the ethynyl group. The latter can thus be used for further reactions and multilayer formation, e.g., by means of alkyne-azide coupling. The observed chemoselective reactivity of ECCO on Si(001) is traced back to the direct reaction channel of cyclooctyne [1] in contrast to the precursor-mediated adsorption pathway of the terminal triple bond.
[1] Reutzel et al., J. Phys. Chem. C **120** 26284 (2016).

O 77.11 Thu 13:00 H9

Phase diagram and order-disorder phase transitions of NTCDA/Ag(111) — •Sebastian Thussing, Martin Grünebohm, and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

A chopped-heating setup has been employed to derive the phase diagram and to follow order-disorder phase transitions of (sub-)monolayer NTCDA on Ag(111). This well-known model system has been chosen to optimize parameters in the experimental setup and to minimize detrimental effects associated with sample heating (direct current heating). We examined 2D SPA-LEED images taken at elevated temperatures as well as 1D line scans obtained during annealing of the molecular layers. NTCDA molecules on Ag(111) experience attractive lateral interactions, leading to island growth already at 150 - 200K for submonolayer coverages. Upon annealing the average NTCDA island size increases steadily (Ostwald ripening) as indicated by an increase of the correlation length of the relaxed monolayer NTCDA LEED reflexes. Further annealing eventually leads to a dissolution of NTCDA islands into the 2D gas phase. The temperature of this transformation depends strongly on the amount of deposited NTCDA. Moreover, this order-disorder transition is preceded by thermal desorption for coverages above 0.55 ML. By analyzing the coverage dependency of the order-disorder phase transition in conjunction with thermal desorption spectroscopy the phase diagram for this system has been derived.

O 78: Electronic Structure of Surfaces I: Photoelectron Spectroscopy

Time: Thursday 10:30–13:15 Location: H14

O 78.1 Thu 10:30 H14

Multidimensional photoemission and the "Inverse LEED State" — •Benedikt Schönhense[1], Katerina Medjanik[2], Sergey Babenkov[2], Dmitry Vasilyev[2], Sergey Chernov[2], Hans-Joachim Elmers[2], and Gerd Schönhense[2] — [1]Imperial College London, Dept. of Bioengineering, UK — [2]Johannes Gutenberg-Universität, Institut für Physik, D-55099 Mainz, Germany

Using a high-energy version of the time-of-flight k-space microscope we recorded $I(E_B, k)$ data arrays at many photon energies in the range of 2.6 to 7 keV at the new hard X-ray beamline P22 at PETRA III (DESY, Hamburg), extending our earlier work at lower energies [1]. Full-field k-imaging of many Brillouin zones (BZs) paves the way to a new type of photoemission experiment, which was impossible with conventional k-microscopes (imaging typically one BZ). The final state in photoemission is a "time-reversed LEED state" [2], since it contains the contribution of all scattering paths experienced by the outgoing electron wave. At keV energies, the valence-band pattern contains substantial contributions from X-ray photoelectron diffraction XPD, which are superimposed on the band features. The results confirm our new model of XPD on the basis of the Laue-equations [3]. The high count rates pave the way towards spin-resolved HAXPES using an imaging spin filter.

[1] K. Medjanik et al., Nature Mat. 16, 615 (2017); [2] S. Hüfner, Photoelectron Spectroscopy, Springer Berlin, (2003); [3] G. Schönhense et al., arXiv: 1806.05871 (2018).

O 78.2 Thu 10:45 H14

Momentum-resolved hard X-ray photoelectron spectroscopy with eliminated diffraction — •S. Babenkov[1], K. Medjanik[1], D. Vasilyev[1], S. Chernov[1], O. Fedchenko[1], C. Schlüter[2], A. Gloskovskii[2], Yu. Matveyev[2], W. Drube[2], B. Schönhense[3], K. Rossnagel[2,4], H.J. Elmers[1], and G. Schönhense[1] — [1]JGU, Inst. für Physik, Mainz — [2]DESY, Hamburg — [3]Imp. Col. London, Dept. of Bioengineering — [4]CAU, Inst. für Exp. und Angew. Physik, Kiel

Hard X-ray angular-resolved photoelectron spectroscopy is a powerful tool to study the electronic band dispersions of buried layers and inner interfaces[1]. Up to now, one had to struggle against experimental obstacles such as low cross-section and strong X-ray photoelectron diffraction (XPD) modulating the spectral density of states. Using a combination of a high-energy version of a time-of-flight k-microscope and the high-brilliance hard X-ray beamline P22 at PETRA III, we are able to acquire full $I(E_B, k)$ data arrays up to hν = 7 keV in short time[2] and thus overcome the previous acquisition time limitations. In order to eliminate the XPD modulation[3] we present a novel method: the normalization of the valence band data by high-resolution core-level XPD patterns, measured at the same kinetic energy and k-field of view, reveal the non-modulated spectral removal function. We present valence band dispersions of molybdenum, graphite and the prototypical dichalcogenide $TiTe_2$ single crystals. [1] A. Gray et al., Nat. Mat. 10, 759 (2011) and Nat. Mat 11, 957 (2012); [2] K. Medjanik et al., Nat. Mat. 16, 615 (2017); [3] G. Schönhense et al., arXiv 1806.05871 (2018).

Invited Talk O 78.3 Thu 11:00 H14

Photoemission of correlated electron pairs from metals excited by megahertz high-order harmonics — •Cheng-Tien Chiang[1,2], Andreas Trützschler[1,2], Michael Huth[2], Robin Kamrla[1,2], Frank O. Schumann[2], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg — [2]Max-Planck-Institut für Mikrostrukturphysik

Electron correlation has been an important topic of solid state physics, which underlies phenomena ranging from magnetism, superconductivity, to metal-insulator transitions. However, direct spectroscopy of correlated electron pairs in solids is a challenging task. By our recent development of laser-based high-order harmonic generation at megahertz repetition rates [1-3] in combination with a pair of time-of-flight spectrometers [4,5], we resolve interacting electron pairs in metals and oxides, and identify their associated valence band character [6]. Our results indicate a band-dependent electron-electron interaction, and the experiments will pave the way towards time- and angle-resolved photoelectron spectroscopy of electron pairs in solids.

[1] C.-T. Chiang, "Angle-resolved photoelectron spectroscopy at surfaces with high-order harmonic generation", Reference module in chemistry, molecular sciences and chemical engineering, edited by K. Wandelt, Elsevier (2018). [2] C.-T. Chiang *et al.*, New J. Phys. **17**, 013035 (2015). [3] C.-T. Chiang *et al.*, J. Electron Spectrosc. Relat. Phenomena, **200**, 15 (2015). [4] M. Huth *et al.*, J. Appl. Phys. **124**, 164504 (2018). [5] M. Huth *et al.*, App. Phys. Lett. **104**, 061602 (2014). [6] A. Trützschler *et al.*, Phys. Rev. Lett. **118**, 136401 (2017).

O 78.4 Thu 11:30 H14

Breakthrough in HAXPES Performance Combining Full-Field k-Imaging with Time-of-Flight Recording — •K. Medjanik[1], S. Babenkov[1], D. Vasilyev[1], S. Chernov[1], O. Fedchenko[1], B. Schönhense[2], C. Schlueter[3], A. Gloskowskii[3], Yu. Matveyev[3], W. Drube[3], H.J. Elmers[1], and G. Schönhense[1] — [1]JGU, Inst. für Physik, Mainz — [2]Imperial College, London — [3]DESY, Hamburg

In order to overcome the intensity/resolution problem of hard X-ray angular-resolved photoelectron spectroscopy (HARPES), we have developed a k-microscope with a modified lens system optimized for high kinetic energies (>7 keV) and very large field of view in k-space (up to 20 $Å^{-1}$ diameter) [1]. First results with this instrument have been taken at the new beamline P22 at PETRA III (Hamburg) [2]. The high X-ray brilliance (1.1x10^{13} hν/s in a spot of $<$ 20x15 μm^2) allows mapping of the 3D bulk Brillouin zone in a few hours. We found that the concept of tomographic k-space mapping previously demonstrated in the soft X-ray regime [3] works equally well in the hard X-ray range. Sharp valence band k-patterns of Re collected at an excitation energy of 6 keV correspond to direct transitions to the 28^{th} repeated Brillouin zone. X-ray photoelectron diffraction (XPD) patterns with $< 0.1°$ resolution are recorded within minutes. The high count rates pave the way towards spin-resolved HAXPES using an imaging spin filter.

[1] K. Medjanik et al., arXiv:1810.11366 (2018); [2] C. Schlueter et al., Synchr. Radiation News 31, 29 (2018); [3] K. Medjanik et al., Nature Materials 16, 615 (2017).

O 78.5 Thu 11:45 H14

The XPS limit within the one-step model of photoemission: temperature and photon energy effects — •Laurent Nicolaï[1], Vladimir Strocov[2], Juraj Krempaský[2], Federico Bisti[2], Charles Fadley[3], Ajith Kaduwela[4], and Ján Minár[1] — [1]Univiversity of West Bohemia, Plzeň, Czech Rep. — [2]Paul Scherrer Institut, Villigen, Suisse — [3]Berkeley, California, USA — [4]University of California, USA

Angle-Resolved Photoemission Spectroscopy (ARPES) is the method of choice for characterising the electronic structure of a given material. A complete understanding of the experimental spectra requires theoretical analyses as well. However, the development of theoretical tools in order to reproduce experimental conditions remains, to this day, a challenge. Using the one-step model of photoemission[1] as implemented in the SPRKKR package[2], our calculations incorporate temperature- and phonon energy-dependent effects via inclusion of both bulk[3] and surface phonons. We also investigate the photon energy range over which the Angle-Integrated PhotoEmission (AIPES) spectra can be compared to the corresponding Weighed Density of States (WDOS).

[1] Braun, Rep. Prog. Phys. 59, 1267-1338 (1996), [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011), [3] L. Nicolaï and J. Minár, AIP Conf. Proc. 1996, 020033 (2018)

O 78.6 Thu 12:00 H14

Impact of collective electrostatic effects on the calculation of core-level excitations within the final state approach — •Thomas C. Taucher, Oliver T. Hofmann, and Egbert Zojer — Institute of Solid State Physics, Graz University of Technology, NAWI Graz, Petersgasse 16, 8010 Graz, Austria

In this contribution we discuss complications arising when applying slab-type density functional theory-based band structure calculations to model core-level excitations at metal-organic interfaces:

When performing calculations using the final state approach, a possible complication is that by exciting an electron in every unit cell, an artificial dipole layer is created. Such dipole layers shift the core-level energies.[1] When adsorbing polar molecules, the shift due to the induced dipole layer is consistent with the actual experimental situation, while in the above mentioned final state calculations, the resulting shifts are artificial.

As a strategy to tackle this issue, we suggest to use larger supercells for the calculations. In this case, the surface coverage stays the same, but only a tiny fraction of the molecules is excited. This approach resembles the actual X-ray photoelectron spectroscopy experiments in a much better way, and is pushing the limitations of today's computational resources.

[1] T. C. Taucher et al., J. Phys. Chem. C, 2016, 120, 3428.

O 78.7 Thu 12:15 H14

The one-step model of 2PPE applied to Co(001) — •Jürgen Braun[1] and Hubert Ebert[2] — [1]Dept. Chemie, LMU München, Germany — [2]Dept. Chemie, LMU München, Germany

Our 2PPE one-step model approach aims at a quantitative description of the time-dependent spectroscopic properties of specific solid systems under consideration, allowing for the inclusion of static correlation effects via the LSDA+DMFT electronic structure approach. To this end we follow Pendry's one-step theory as close as possible and make extensive use of concepts of relativistic multiple-scattering theory within the LKKR method in order to guarantee for angular resolution in the spectroscopic calculations [1]. The fully relativistic formalism has been applied to fcc Co(001). We discuss our results in context with corresponding experimental data [2].

[1] J. Braun, and H. Ebert, Relativistic theory of 2PPE from ferromagnetic materials, Phys. Rev. B (2018), (submitted)

[2] A. B. Schmidt, M. Pickel, T. Allmers, M. Budke, J. Braun, M. Weinelt, and M. Donath, Spin-dependent surface electronic structure of fcc Co films, J. Phys. D: Apl. Phys. **41**, 164003 (2008)

O 78.8 Thu 12:30 H14

Electronic properties of Cobalt-Pyrphyrin on Cu_2O(111) - A model electrode for photocatalytic water splitting — •Lisa Grad, Adrian Schuler, Matthias Hengsberger, and Jürg Osterwalder — University of Zurich, Physics Institute, Winterthurerstrasse 190, 8057 Zurich, Switzerland

Photocatalytic water splitting represents a sustainable way to store solar energy in the form of chemical bonds. For large-scale use, the combination of molecular catalysts supported on light absorbing substrates is a viable approach.

With photoemission experiments we investigate the electronic properties of one model cathode consisting of the metalorganic molecule Cobalt-Pyrphyrin (CoPyr) adsorbed on the Cu_2O(111) surface. Due to its small band gap Cu_2O(111) is an efficient photoabsorber for solar light. Further it is a p-type semiconductor with downward band bending towards the surface. With angle-resolved X-ray photoelectron spectroscopy the band bending close to the surface could be determined before and after the adsorption of CoPyr molecules.

The related electric field leads to charge separation of photogenerated electron-hole pairs. By means of time-resolved two-photon photoemission we could determine the relaxation dynamics and the lifetime of photo-excited electrons in the conduction band of pristine Cu_2O(111).

Our current work is focused on the investigation of the energy level alignment, the charge injection into and the lifetime of electrons in the molecular states of CoPyr adsorbed on Cu_2O(111).

O 78.9 Thu 12:45 H14

Investigating the surface composition of perfluorofunctionalized ionic liquid mixtures by angle-resolved X-ray photoelectron spectroscopy — •Bettina Heller[1], Matthias Lexow[1], Gabriel Partl[2], Hans-Peter Steinrück[1], and Florian Maier[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Institut für Allgemeine, Anorganische und Theoretische Chemie, Leopold-Franzens-Universität Innsbruck, Innsbruck, Austria

Due to their extremely low vapor pressure, ionic liquids (ILs) -salts with a melting point below 100 °C per definition- can be investigated under ultra-high vacuum (UHV) conditions with angle-resolved X-ray photoelectron spectroscopy (ARXPS). Using a unique "Dual Analyzer System for Surface Analysis" (DASSA)[1], simultaneous ARXP spectra taken in 0° (bulk sensitive) and 80° (surface sensitive) emission relative to the surface normal provide detailed information about composition and molecular orientation at the sample surface.[2]

In this work, temperature-dependent XPS measurements of IL mixtures consisting of 1-alkyl-3-methylimidazolium hexafluorophosphate $[\mathrm{C}_n\mathrm{C}_1\mathrm{Im}][\mathrm{PF}_6]$ and a perfluoro-functionalized IL will be presented, showing a more pronounced surface enrichment of the perfluoro-chain at lower temperature.

[1] I. Niedermaier, C. Kolbeck, H.-P. Steinrück, F. Maier, *Rev. Sci. Instrum.* **2016**, *87*, 045105.

[2] H.-P. Steinrück, *Phys. Chem. Chem. Phys.* **2012**, *14*, 5010.

O 78.10 Thu 13:00 H14

Dirac nodal lines and flat-band surface state in the functional oxide RuO2 — Vedran Jovic[1,2], Roland J. Koch[1], Swarup K. Panda[3], Helmuth Berger[4], Philippe Bugnon[4], Arnaud Magrez[4], Kevin E. Smith[2,5], Silke Biermann[3,6], Chris Jozwiak[1], Aaron Bostwick[1], Eli Rotenberg[1], and •Simon Moser[1,7] — [1]Advanced Light Source — [2]Auckland University — [3]Ecole Polytechnique — [4]EPFL — [5]Boston University — [6]College de France — [7]Würzburg University

The efficiency and stability of RuO2 in electro-catalysis has made this material a subject of intense fundamental and industrial interest. The surface functionality is rooted in its electronic and magnetic properties - determined by a complex interplay of lattice-, spin-rotational, and time-reversal symmetries, as well as the competition between Coulomb- and kinetic energies. This interplay was predicted to produce a network of Dirac nodal lines (DNL), where the valence- and conduction bands touch along continuous lines in momentum space. Here we uncover direct evidence for three DNLs in RuO2 by angle resolved photoemission spectroscopy (ARPES). These DNLs give rise to a flat-band surface state (FBSS) that is readily tuned by the electrostatic environment, and that presents an intriguing platform for exotic correlation phenomena. Our findings support high spin- Hall conductivities and bulk magnetism in RuO2, and are likely related to its catalytic properties.

O 79: Focus Session: Spins on Surfaces I (joint session O/MA)

Organizer: Andreas Heinrich (Center for Quantum Nanoscience, IBS, Seoul, South Korea)

Time: Thursday 10:30–13:00 Location: H15

Invited Talk O 79.1 Thu 10:30 H15

Enhancing quantum coherence of magnetic atoms on a surface — •Yujeong Bae[1,2,3], Kai Yang[2], Philip Willke[1,3], Taeyoung Choi[1,3], Andreas J. Heinrich[1,3], and Christopher P. Lutz[2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul 03760, Republic of Korea — [2]650 Harry Rd — [3]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea

Coherent control of spin states is of central importance in spin-based information processing and spintronic devices. However, the spin coherence of individual atoms on a surface is easily disrupted by interaction with environment such as electric or magnetic field noise as well as unwanted coupling with neighboring spins. Here we demonstrate that a singlet-triplet transition in a pair of antiferromagnetically coupled spin-1/2 atoms yields enhanced spin coherence compared to individual atoms. We used scanning tunneling microscope to assemble two hydrogenated titanuim atoms on MgO(001). At a precisely selected spacing that gives a large interaction energy between two atoms, we obtain spin states having a high degree of protection from disrupting fields, and also provides thermal initialization into the singlet state. We show that a two level system composed of these singlet and triplet states is insensitive to global and local magnetic field variation, resulting in longer spin coherence times compared to individual atoms.

O 79.2 Thu 11:00 H15

Quantum Nanoscience: Atoms on Surfaces as Quantum Spins — •Andreas Heinrich — IBS Center for Quantum Nanoscience at Ewha Womans University, Seoul, Korea

Quantum Nanoscience is a discipline that combines quantum science with nanoscience. It aims to utilize quantum coherence in solid-state and molecular systems. Among the many basic science questions in this field are open versus closed quantum systems and the controlled interaction of the quantum systems with the host materials. Getting control of those methods and concepts will enable engineered quantum systems with controllable quantum coherence. Possible applications range from quantum sensing to quantum computation. Scanning Tunneling Microscopy is a unique tool in that it allows to image surface with atomic resolution, build structures one atom at a time and measure the structures with high energy and spin resolution - all in one machine. We will outline relevant experiments that enable the STM to become a potent tool of quantum nanoscience.

O 79.3 Thu 11:15 H15

Sensing the spin of a spectroscopically dark Ce adatom with an STM — •Markus Ternes[1,2], Chris Lutz[3], Andreas Heinrich[4,5], and Wolf-Dieter Schneider[6,7] — [1]RWTH Aachen University, Germany — [2]Peter Grünberg Institute PGI-3, Forschungszentrum Jülich, Germany — [3]IBM Almaden Research Center, San Jose, CA, USA — [4]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea — [5]Ewha Womans University, Seoul, Republic of Korea — [6]Fritz- Haber-Institut, Berlin, Germany — [7]École Polytechnique Fédérale de Lausanne, Switzerland

The magnetic moment of rare earth elements originates from the electrons of the partially filled $4f$ orbitals. Accessing this moment electrically as in a scanning tunneling spectroscopy experiment is difficult due to the effective shielding by electrons in the further outward lying $5d$ and $6s$ orbitals. However, recently the influence of $4f$ spins on the EPR signal of neighboring $3d$ spins has been used for its detection [1]. Here we use a different approach to detect the magnetic moment of a single Ce adatom on a $\mathrm{Cu_2N}$ ultrathin film on Cu(100). We functionalize the tip apex with a second, Kondo screened spin which we can deliberately couple to other moments on the surface via the tunneling junction [2]. We calibrate this sensor against a well understood Fe atom and subsequently use the splitting of the Kondo resonance when approaching a spectroscopically dark Ce atom to determine its magnetic moment to $\approx 1\mu_B$. [1] F. D. Natterer, *et al.*, *Nature* **543**, 226 (2017). [2] M. Muenks, *et al.*, *Nature Comm.* **8**, 14119 (2017).

O 79.4 Thu 11:30 H15

Scanning tunneling spectroscopy of Co atoms at long Cu chains — Neda Noei[1], •Alexander Weismann[1], Roberto Mozara[2], Oleg Kristanovski[2], Alexander I. Lichtenstein[2], and Richard Berndt[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

The interaction of an impurity atom carrying a localized spin with a host metal often leads to the many-body Kondo effect. We prepared atomic chains with lengths of hundreds of Cu atoms on a Cu(111) surface, and spectroscopically probed the Kondo resonance of Co adatoms on pristine terraces, at such chains, and at the end of chains. Distinctly different amplitudes, widths and spectroscopic line shapes are observed for the three cases and they are qualtatively reproduced by multi-orbital many body calculations that combine DFT with continuous-time quantum Monte Carlo.

O 79.5 Thu 11:45 H15

Spin selective tunneling processes between Yu-Shiba-Rusinov states — •Haonan Huang[1], Jacob Senkpiel[1], Robert Drost[1], Ciprian Padurariu[2], Simon Dambach[2], Björn Kubala[2], Juan Carlos Cuevas[3], Alfredo Levy Yeyati[3], Joachim Ankerhold[2], Christian R. Ast[1], and Klaus Kern[1,4] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]Institut für komplexe Quantensysteme, Universität Ulm, Ulm, Germany — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain — [4]EPFL, Switzerland

A Yu-Shiba-Rusinov (YSR) state is a pair of in-gap states resulting from the interaction of magnetic atoms with a superconductor. We are experimentally able to introduce any YSR state of desired energy position and peak heights to the apex of a superconducting vanadium

STM tip, and then use this novel tip to characterize sample YSR defects to study spin selective tunneling. YSR-YSR tunneling happens resonantly when the bias voltage is at the sum of tip and sample YSR energies. If the temperature is finite, there is thermal occupation of the originally empty YSR state, which results in thermally assisted YSR-YSR tunneling that happens at the difference of tip and sample YSR energies. The relative spin orientation will change the intensity of both processes, and Green's function theory can readily explain the spin selection rules. We use a mK-STM to study the YSR-YSR tunneling processes from 15mK to 1K, and the temperature dependence of thermal and normal YSR-YSR processes gives insight of their spin dynamics.

O 79.6 Thu 12:00 H15

Integrating Yu-Shiba-Rusinov states into a tunnel junction — •Christian R. Ast[1], Haonan Huang[1], Jacob Senkpiel[1], Robert Drost[1], Simon Dambach[2], Ciprian Padurariu[2], Björn Kubala[2], Juan Carlos Cuevas[3], Alfredo Levy Yeyati[3], Joachim Ankerhold[2], and Klaus Kern[1,4] — [1]MPI für Festkörperforschung, Stuttgart — [2]Institut für komplexe Quantensysteme, Universität Ulm, Ulm — [3]Universidad Autónoma de Madrid, Madrid, Spain — [4]EPFL, Lausanne, Switzerland

Magnetic impurities in a superconductor give rise to subgap features called Yu-Shiba-Rusinov (YSR) states. On or near surfaces, these impurities can be well studied locally by scanning tunneling microscopy (STM). We have observed a non-trivial energy dependence of the YSR state as a function of tip-sample distance, similar to findings that have been reported before. The occurrence of this phenomenon deep in the tunneling regime suggests a non-negligible influence of the tip on the YSR impurity. Therefore, in order to interpret this energy dependence, a more holistic model of the tunnel junction including the YSR state is necessary. To this end, we discuss a model that extends the existing Green's function description of YSR states and also bridges a gap to related models.

O 79.7 Thu 12:15 H15

Interplay between Yu-Shiba-Rusinov states and spin-flip excitations on magnetic impurities on superconducting NbSe$_2$ substrate — •Shawulienu Kezilebieke[1], Rok Žitko[2], Marc Dvorak[1], Teemu Ojanen[3], and Peter Liljeroth[1] — [1]Department of Applied Physics, Aalto University School of Science, 00076 Aalto, Finland — [2]Jožef Stefan Institute, Jamova 39, SI-1001 Ljubljana, Slovenia — [3]Laboratory of Physics, Tampere University of Technology, Tampere FI-33101, Finland

Exchange coupling between a magnetic impurity and a superconducting substrate results in the formation of Yu-Shiba-Rusinov (YSR) bound states, which have been recently used in artificial designer structures to realize exotic quasiparticles known as Majorana fermions. At strong coupling, the energies of YSR states are deep in the superconducting gap. At weak coupling, the YSR states migrate towards the superconducting gap edge. Additional spectral features can appear in the presence of magnetic anisotropy with spin $S \geqslant 1$, in particular spin-flip excitations outside the superconducting gap. Despite extensive experiments on magnetic impurities that exhibit separately either spin-flip excitations or YSR states, these phenomena have not been observed simultaneously. Here, we investigate the spectral evolution in different metal phthalocyanine molecules on NbSe$_2$ surface as a function of the coupling with the substrate. Using scanning tunneling microscopy (STM), we tune the exchange coupling strength and for manganese phthalocyanine (MnPc) we demonstrate a smooth spectral crossover from the YSR states to intrinsic quantum spin states.

O 79.8 Thu 12:30 H15

Fractional charge tunneling between Shiba states in STM devices — •Ciprian Padurariu[1], Haonan Huang[2], Björn Kubala[1], Simon Dambach[1], Christian R. Ast[2], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, 89069 Ulm, Germany — [2]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

We present the theory and experimental realization of tunneling between tip and substrate Shiba states in superconducting STM devices operating at 15 mK. The simple analytical results are in good agreement with conductance measurements exhibiting peaks in the tunnel current at a number of sub-gap bias voltages. [1] The voltages are identified as resonances of sub-gap discrete magnetic states, so called Shiba states, that form inside a volume around the magnetic impurity of coherence length size. [2]

When a Shiba state formed around an impurity in the STM tip is brought into proximity with a Shiba state formed around an impurity in the substrate, new resonances arise at characteristic values of the voltage. The tunnel current at the new resonances is a result of the interplay between coherent transport processes and incoherent relaxation. The elementary transport process carries a fractional charge proportional to the electron-hole asymmetry in the device.

[1] M. Ruby, F. Pientka, Y. Peng, F. von Oppen, B. W. Heinrich, and K. J. Franke, Phys. Rev. Lett. **115**, 087001 (2015).

[2] M. I. Salkola, A. V. Balatsky, and J. R. Schrieffer, Phys. Rev. B **55**, 12648 (1997).

O 79.9 Thu 12:45 H15

Renormalization of single-ion magnetic anisotropy by charge fluctuations — •David Jacob — Dpto. de Física de Materiales, Universidad del País Vasco UPV/EHU, San Sebastián, Spain — IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Inelastic spin-flip excitations associated with single-ion magnetic anisotropy of quantum spins can be strongly renormalized by Kondo exchange coupling to the conduction electrons in the substrate, as shown recently for the case of Co adatoms on CuN$_2$ islands [1]. In this case, differential conductance spectra show zero-bias anomalies due to a Kondo effect of the doubly degenerate ground state, and finite-bias step features due to spin-flip excitations. Here I consider spin-1 quantum magnets with positive uniaxial anisotropy, where the ground state is nondegenerate and hence the Kondo effect does not take place [2]. Nevertheless, despite the absence of Kondo effect the magnetic anisotropy can still be strongly renormalized, both by exchange coupling to the conduction electrons and also by charge fluctuations. Interestingly, in contrast to the renormalization by Kondo exchange, charge fluctuations lead to asymmetric spectra, which, for strong charge fluctuations, mimic Fano-Kondo lineshapes, even though the origin is completely different.

References: [1] J. C. Oberg *et al.*, Nature Nanotechnol. **9**, 64 (2014); [2] D. Jacob, Phys. Rev. B **97**, 075428 (2018)

O 80: Ultrafast Electron Dynamics at Surfaces and Interfaces I

Time: Thursday 10:30–13:00 Location: H16

O 80.1 Thu 10:30 H16

Ultra-fast core-level dynamics in semiconducting WSe$_2$ — •Maciej Dendzik[1], R. Patrick Xian[1], Dmytro Kutnyakhov[2], Shuo Dong[1], Federico Pressacco[3], Davide Curcio[4], Steinn Agustsson[5], Michael Heber[2], Jasper Hauer[1], Wilfried Wurth[2,3], Günter Brenner[2], Yves Acremann[6], Philip Hofmann[4], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14915 Berlin, Germany — [2]DESY Photon Science, Notkestr. 85, 22607 Hamburg, Germany — [3]CFEL, Hamburg University, Luruper Chausee 149, 22761 Hamburg, Germany — [4]Aarhus University, 8000 Aarhus C, Denmark — [5]JGU Mainz, Staudingerweg 7, 55128 Mainz, Germany — [6]ETH Zurich, Otto-Stern-Weg 1, 8093 Zurich, Switzerland

The development of femtosecond XUV sources such as the Free-Electron Laser FLASH [1] combined with recent improvements of electron detection (momentum microscopy [2]) enables studying ultra-fast processes governing the excitations of core-level electrons. Here we present a study of femtosecond dynamics of W4f core levels in semiconducting WSe$_2$. We find that pumping A-exciton at 800 nm induces changes of both position and shape of observed spectra. In particular, we find a distinct change of the symmetric Lorentzian line profile into a metal-like Doniach-Šunjić asymmetric line shape. We follow the time evolution of induced changes and compare it with the dynamics of valence electrons. [1] W. Ackermann et al., Nat. Phot. 1, 336-342(2007) [2] S.V. Chernov et al., Ultramicroscopy 159, 453-463(2015)

O 80.2 Thu 10:45 H16

Practical Limitations of Floquet Topological Insulators — •Sven Aeschlimann[1], Mariana Chavez-Cervantes[1], Razvan Krause[1], Camilla Coletti[2], Kai Rossnagel[3], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany — [2]Center for Nanotechnology @ NEST, Istituto Italiano di Tecnologia, Pisa, Italy — [3]Institute of Experimental and Applied Physics, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

Recently, using Floquet theory, Oka and Aoki [1] realized that graphene illuminated by circularly polarized light provides and experimental realization of the Haldane model [2] that predicts the occurrence of a quantum Hall effect in the absence of magnetic fields. We used time- and angle-resolved photoemission spectroscopy to search for the predicted Floquet sidebands, changes of the photoemission matrix element due to the induced non-zero z-component of the pseudospin, and band gap opening [3]. After careful optimization of all experimental parameters we observed Floquet sidebands in cleaved bulk WSe2 crystals but not in epitaxial graphene. We attribute the absence of Floquet effects in graphene to scattering times that are short compared to the period of the driving field. Our results have important implications for the experimental realization of Floquet topological insulators and related proposals [4].

[1] T. Oka and H. Aoki, PRB 79, 081406 (2009) [2] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988) [3] M. A. Sentef et al., Nat. Commun. 6, 7047 (2015) [4] M. Claassen et al., Nat. Commun. 7, 13074 (2016)

O 80.3 Thu 11:00 H16

Valley-polarized excitation in singly-oriented monolayer WS_2/Au(111) — •Hauke Beyer[1], Gerald Rohde[1], Antonija Grubisic Cabo[2], Ankatrin Stange[1], Luca Bignardi[3], Daniel Lizzit[3], Paolo Lacovig[3], Silvano Lizzit[3], Kai Rossnagel[1], Philip Hofmann[2], and Michael Bauer[1] — [1]IEAP, Kiel University, Germany — [2]Department of Physics and Astronomy, Aarhus University, Denmark — [3]Elettra Sincrotrone Trieste, Italy

Time- and angle-resolved photoelectron spectroscopy (trARPES) is employed to study the valley-selective excitation and near-surface dynamics of carriers in singly-oriented monolayer WS_2/Au(111). Upon photoexcitation with circularly polarized light ($\lambda \approx 590\,\text{nm}$), we observe a selective population of both valence and conduction band at K and K′, respectively. Our results are consistent with the fraction of domains with mirror orientation being $\leq 10\,\%$, a value that was determined in diffraction experiments [1]. The quantitative analysis of the data indicates a valley polarization in the valence band of $\approx 90\,\%$, while in the conduction band the valley polarization only reaches values of $\approx 70\,\%$. We explain this difference by the small spin-orbit splitting of the conduction band, which promotes intervalley scattering processes. Different carrier dynamics of valence and conduction band population further hint to intervalley scattering being of relevance for the depolarization of the conduction band.

[1] Luca Bignardi et al., arXiv:1806.04928v2

O 80.4 Thu 11:15 H16

Interplay between CDW quenching and the excited phonon population in TiSe_2, observed via ultrafast transmission electron diffraction — •William WINDSOR[1], Daniela Zahn[1], Helen Seiler[1], Ralph Ernstorfer[1], Laurenz Rettig[1], and Kai Rossnagel[2] — [1]Fritz-Haber-Institut der MPG (DE) — [2]University of Kiel (DE)

TiSe2 is a 2D material which exhibits a charge density wave (CDW) below 200K, with a CDW-driven energy gap of 0.4eV. Here we study ultrafast structural dynamics of the CDW phase following a mid-IR excitation, slightly above the gap. We observe the quenching of the CDW, followed by Subsequent dynamics of the lattice, and a varying excited population of high- and low-wavevector phonons within the inelastic background. Dynamics of the CDW, the lattice and the inelastic background will be comparatively discussed.

O 80.5 Thu 11:30 H16

Real-space order parameter mapping using ultrafast transmission electron microscopy — •Thomas Danz, Till Domröse, and Claus Ropers — 4th Physical Institute – Solids and Nanostructures, University of Göttingen, Germany

Over the past decades, ultrafast optical techniques have considerably shaped our understanding of homogeneous materials, while transmission electron microscopy has greatly contributed to elucidating atomic structures and compositions on the sub-nanometer scale. Combining these concepts, ultrafast transmission electron microscopy (UTEM) allows for resolving femtosecond dynamics in heterogeneous materials using imaging, diffraction, and spectroscopy [1].

The pulsed electron source of the Göttingen UTEM project employs linear photoemission from a nanoscopic Schottky emitter, delivering highly coherent electron pulses with down to 200 fs pulse duration, 0.6 eV energy width, and sub-1 nm focused beam diameter [2].

Here, we demonstrate the ultrafast real-space mapping of the order parameter for a charge-density wave phase transition in the correlated material 1T-TaS_2. Specifically, we track the evolution of domain patterns on femtosecond to picosecond time and nanometer length scales, extracting characteristic observables not accessible by ultrafast electron or x-ray diffraction.

[1] A. H. Zewail, Science **328**, 187 (2010).

[2] A. Feist, Th. Danz *et al.*, Ultramicroscopy **176**, 63 (2017).

O 80.6 Thu 11:45 H16

Atomically-resolved ultrafast dynamics in CDW-Mott-insulator materials — •Shaoxiang Sheng[1], Mohamad Abdo[1,2,3], Moritz Tritschler[1], Luigi Malavolti[1,2,3], Max Hänze[1,2,3], Gregory McMurtrie[1,2,3], Lukas Arnhold[1], and Sebastian Loth[1,2,3] — [1]Universität Stuttgart, Institut für Funktionelle Materie und Quantentechnologien, Stuttgart, Germany — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Electron-electron interaction plays an important role in strongly correlated systems. This may drive the electrons near the Fermi surface to localize resulting in a metal-to-insulator transition. Layered 1T-TaS2, as a model system, presents rich electronic properties, which go through a series of charge-density wave (CDW) phases into a Mott insulating ground state as the temperature decreases.[1] By combining THz pump-probe spectroscopy and low-temperature scanning tunneling microscopy (STM), we can study ultrafast electron dynamics of the Mott phase at the atomic scale. The pump-probe spectra vary strongly on the scale of one unit cell of the CDW. The results shed new light onto the microscopic dynamics of electron motion in the Mott phase.

[1] Sipos, B., et al. Nature Materials 7, 960-965 (2008).

O 80.7 Thu 12:00 H16

Probing non-equilibrium lattice excitations in 1T-TaS2 by ultrafast LEED — •Gero Storeck[1], Theo Diekmann[1], Gerrit Horstmann[1], Simon Vogelgesang[1], Kai Rossnagel[2], and Claus Ropers[1] — [1]4th Physical Institute - Solids and Nanostructures, University of Göttingen, Germany — [2]Institute for Experimental and Applied Physics, University of Kiel, Germany

Transition-metal dichalcogenides (TMDCs) exhibit a multitude of correlation-induced states, such as charge-density wave (CDW) phases coupled to a periodic lattice distortion (PLD). Optical excitation of these states leads to a transient quench of the CDW gap and the excitation of various fluctuation modes. While the Raman-active amplitude modes lead to strong signatures in optical spectroscopy and are frequently observed in photoelectron spectroscopy, phason excitations remain more elusive [1,2].

Here, we present an ultrafast low-energy electron diffraction (ULEED) study of the incommensurate and nearly commensurate CDW phases of 1T-TaS_2 [3]. We trace the non-equilibrium dynamics of the CDW amplitude, and study the population of phonon and phason modes by their influence on the diffraction intensity of the lattice Bragg peaks, the PLD satellite peaks as well as the diffuse background scattering.

[1] Lee, W. S. et al., Nature Communications 3, (2012).

[2] Liu, H. Y. et al., Physical Review B 88, (2013).

[3] Wilson et al., Advances in Physics 24, 117-201 (1975).

O 80.8 Thu 12:15 H16

Ultrafast exciton dynamics in monolayer WS2 probed by femtosecond time-resolved (non-)linear optical spectroscopies. — •Stefano Calati[1], Selene Mor[1], Sarah King[1,2], and Julia Stähler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (DE) — [2]University of Chicago, Department of Chemistry, Chicago, USA

Controlling the optical properties of transition metal dichalcogenides (TMDCs) on ultrashort timescale is foundamental for device applications. Our aim is to unveil the foundamental processes responsible for the exciton dynamics of these materials. We present our work on pristine monolayer WS2 using femtosecond time-resolved reflectivity contrast (tr-RC) and electronic sum frequency generation (tr-eSFG) optical spectroscopies [1]. We present tr-RC measurements of monolayer WS2 with unprecedented time resolution. We discover an unexpected transient blueshift of the A excitonic resonance, which depends on the excitation density and photon energy. We identify and discuss the ultrafast processes responsible for the observed dynamics. Furthermore, we report intense eSFG generation from a monolayer WS2. We identify a resonant contribution of the A exciton, and the transient changes are compared to the dynamics observed in the linear optical experiment. These studies provide the basic framework for future studies on energy and charge transfer at TMDC-based hybrid interfaces.

[1] L. Foglia et al., Appl. Phys. Lett. 109, 202106 (2016)

O 80.9 Thu 12:30 H16

Inter- and intralayer electron dynamics in MoS_2 probed by 2PPE — •Robert Wallauer, Johannes Reimann, Jens Güdde, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, 35037 Marburg

We use time- and angle-resolved two photon photoemission (2PPE) with a high-harmonic probe for the investigation of electron dynamics of MoS_2 in momentum space. For this purpose, we combined a high-repetition rate high-harmonic source with a 3D (k_x, k_y, E) electrostatic electron spectrometer [1]. The pump laser is tunable within the visible from around 500 - 700 nm. At our high-harmonic photon energy of 23.5 eV we essentially probe only the first layer, which differs from the bulk with respect to band energies.

By tuning our pump laser above and below the band gap of the first layer we are able to selectively induce the excitation from the valence into the conduction band at $\overline{K}$ within the first layer or alternatively in deeper layers. For all photon energies, the relaxation to the conduction band minimum at $\overline{\Sigma}$ is observed. The relaxation dynamics, however, varies with pump photon energy, which allows us to distinguish between charge transfer within the first layer and charge transfer between adjacent layers.

[1] R. Wallauer et al., Appl. Phys. Lett. 109, 162102 (2016).

O 80.10 Thu 12:45 H16

Decoding the Ultrafast Formation of a Fermi-Dirac Distributed Electron Gas — •Gerald Rohde, Ankatrin Stange, Arne Müller, Marcel Behrendt, Lars Oloff, Kerstin Hanff, Hauke Beyer, Thies Albert, Petra Hein, Kai Rossnagel, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

A photoexcited electron gas is phenomenologically often described within multitemperature models, which consider the electronic system being internally thermalized for all times. Ultrafast nonthermal phenomena taking place right after photoexcitation are still largely unexplored. Time- and angle-resolved photoemission spectroscopy operated near the Fourier-limit and at a temporal resolution of ≈10 fs is used to sample the ultrashort time frame of 50 fs in the formation of a Fermi-Dirac distributed electron gas in graphite following an impulsive photoexcitation [1]. We identify and dissect experimentally characteristic stages associated with different interaction processes among the involved degrees of freedom, which have been predicted theoretically in the past [2,3]. The scenario involves electron-photon, electron-electron, and electron-phonon interaction affecting the response of the system on different timescales. Our results reveal experimentally the complexity of the transition from a nascent nonthermal towards a thermal electron distribution in a graphitic material with reduced screening.

[1] G. Rohde *et al.*, Phys. Rev. Lett. *accepted* (2018)
[2] M. Mittendorff *et al.*, Nano Lett. 14, 1504 (2014)
[3] T. Winzer *et al.*, J. Phys. Condens. Matter 25, 054201 (2013)

O 81: Gerhard Ertl Young Investigator Award

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

Invited Talk O 81.1 Thu 10:30 H24

Zooming in on the electronic properties of van der Waals Heterostructures — •Søren Ulstrup[1], Jyoti Katoch[2], Roland J. Koch[3], Simon Moser[3], Kathleen M. McCreary[4], Simranjeet Singh[2], Jinsong Xu[2], Berend T. Jonker[3], Roland K. Kawakami[2], Aaron Bostwick[3], Eli Rotenberg[3], and Chris Jozwiak[3] — [1]Department of Physics and Astronomy, Aarhus University, DK — [2]Department of Physics, Ohio State University, USA — [3]Advanced Light Source, Berkeley Lab, USA — [4]Navel Research Lab, USA

Two-dimensional (2D) semiconducting transition metal dichalcogenides (TMDs) exhibit a diverse collection of intriguing electronic phenomena. These include single-particle effects related to new spin and valley physics, as well as exotic many-body interactions. The latter are exemplified by the presence of tunable band gaps and tightly bound excitons and trions. Here, I will show how the electronic properties of complex heterostructures composed of tungsten disulfide and boron nitride (WS_2/hBN) can be accessed using angle-resolved photoemission spectroscopy with nano-scale spatial resolution (nanoARPES). I will present three major discoveries in such stacks: (i) The direct observation of the energy- and momentum-dependent electronic structure of one-dimensional TMD nanoscrolls, (ii) a substrate-induced lateral band bending, demonstrating ultimate control of band offsets at the nanoscale, and (iii) a doping dependent three-particle excitation in the measured spectral function which is consistent with the formation of a trion.

Invited Talk O 81.2 Thu 11:00 H24

Directly measuring the anisotropic magnetic exchange force field of a spin spiral — •Nadine Hauptmann[1], Tzu-Chao Hung[1], Wouter Jolie[1], Soumyajyoti Haldar[2], Daniel Wegner[1], Stefan Heinze[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, Netherlands — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Chiral magnets, e.g. magnetic skyrmions and spin spirals, are hot candidates for nano-scale magnetic storage. These magnetic structures are stabilized by an interplay between competing exchange interactions at the atomic-scale. Spin-polarized scanning tunneling microscopy (SP-STM) has achieved great success in investigating the magnetization of such structures, but faces a number of limitations in being able to directly detect the underlying exchange forces, as well delineate between structural and electronic contributions to the spin-polarized density of states. To go beyond these limitations, we have developed a new method, which combines SP-STM and magnetic exchange force microscopy (SPEX) based on nc-AFM utilizing a tuning fork design. The method has been successfully applied to independently determine the structural corrugation from the electronic and magnetic contributions for single and bi-layers of Fe/Ir(111). Here, we investigate a new regime for SPEX, namely characterize the distance-dependent spectroscopy of the noncollinear magnetic exchange force derived from the antiferromagnetic spin spiral in a monolayer Mn/W(110).

Invited Talk O 81.3 Thu 11:30 H24

Scanning Probe Microscopy at Ambient Pressures — •Baran Eren — Department of Chemical and Biological Physics, Weizmann Institute of Science, 234 Herzl Street, Rehovot, Israel

We perform surface science studies in the presence of gases, while avoiding significant sacrifices in terms of measurement resolution and accuracy. This involves microscopy and spectroscopy techniques that have been specially adapted to be performed at ambient pressures. Atomic structure and chemical properties of low Miller-index Cu surfaces exposed to CO, CH3OH, and CO2 will be presented. Cu surfaces break up into nanoclusters at RT in the presence of CO in the Torr pressure range. This finding has implications in heterogeneous catalysis as it shows how the surface evolves, affecting its electronic structure and chemical properties. The reason behind clustering is the high difference in adsorption energy of CO on low-coordinated Cu atoms as compared to high-coordinated Cu atoms. In addition, adsorbed CO weakens the binding of the Cu atom to its neighbors, which facilitates the detachment of the edge Cu atoms and their diffusion. Unlike CO, CH3OH does not cause the break-up of Cu into clusters because methoxy adsorbs strongly both on step and terrace atoms.

STM is limited to electrically conducting surfaces but many real catalysts are supported on insulating oxides. We built an AFM system to operate under reactant gases, and we are developing a new methodology to use Hamaker constants to obtain chemical fingerprints at the lower nanometer scale.

Invited Talk O 81.4 Thu 12:00 H24

High energy surface x-ray diffraction from surfaces and particles in operando catalysis — •Uta Hejral[1], Stefano Albertin[1], Mikhail Shipilin[2,3], Jianfeng Zhou[1], Sebastian Pfaff[1], Sara Blomberg[1], Johan Zetterberg[1], Johan Gustafson[1], Andreas Stierle[2], and Edvin Lundgren[1] — [1]Lund University, Lund, Sweden — [2]DESY, Hamburg, Germany — [3]Stockholm University, Stockholm, Sweden

Catalysts are widely employed in chemical industry, in fuel cells and car exhaust control systems, where they accelerate desired chemical reactions. To improve catalyst performance, a time-resolved atomic-scale understanding of the interplay between the catalyst surface structures, the catalytic activity/selectivity, and the gas phase surrounding the catalyst surface is inevitable.

High energy surface x-ray diffraction (HESXRD) provides a fast data acquisition for the structural characterization of model catalyst samples under operando conditions. We demonstrate how we used HESXRD to study the shape-dependent sintering of supported Pt-Rh alloy nanoparticles during CO oxidation. Flat-shaped Pt-rich particles underwent strong vertical sintering, while Rh-rich compact-shaped particles proved to be sinter-resistant. In another experiment we combined HESXRD with gas phase diagnostics to investigate the structure-gas phase correlation during self-sustained reaction oscillations over Pd(100) during CO oxidation. We found that the surface features epitaxial PdO(101) bulk oxide decorated by metallic Pd islands on top, which play a crucial role for the self-sustained oscillations.

Invited Talk O 81.5 Thu 12:30 H24

Batteries at Work: Towards Operando Photoelectron Spectroscopy on Lithium Ion Batteries — •Julia Maibach[1,2], Ida Källquist[3], Kristina Edström[2], Håkan Rensmo[3], Hans Siegbahn[3], and Maria Hahlin[3] — [1]Karlsruhe Institute of Technology, Institute for Applied Materials, Germany — [2]Uppsala University, Department of Chemistry - Ångström Laboratory, Sweden — [3]Uppsala University, Department of Physics and Astronomy, Sweden

Almost 40 years after the first commercially available lithium ion battery, the solid electrolyte interphase (SEI) is still considered one of the least understood parts in a lithium ion battery. While it is known that the SEI forms from decomposition products of the liquid battery electrolyte on the negative electrode, the exact formation mechanism and this results in the functionality of an electrode protection layer with Li ion conductivity are not yet fully understood. In this presentation, we will first discuss the challenges of SEI characterization and then present our approach to operando ambient pressure x-ray photoelectron spectroscopy (AP-XPS) on lithium ion battery systems. This technique can provide the key tool that has been missing so far to probe the functionality of the electrode/electrolyte interface in more realistic battery environments. We will show our results of AP-XPS characterizations of liquid carbonate-based battery electrolytes, battery electrodes with the liquid electrolyte present, and how the electrochemical reactions of a battery can be driven and followed under the measurement conditions pertaining to photoelectron spectroscopy.

O 82: Fundamentals of Catalysis II

Time: Thursday 15:00–17:45 Location: H5

O 82.1 Thu 15:00 H5

Embedding of cluster superlattices to prevent sintering — •Tobias Hartl, Moritz Will, Pantelis Bampoulis, and Thomas Michely — II. Physikalische Institut, Universität zu Köln

Deposition of a metal, for example Ir, Pt, or W, on the moiré of Gr on Ir(111) leads to a well-ordered cluster superlattice [1]. These clusters are tunable in size, from a few up to hundreds of atoms each, and are of interest for catalysis due to their size dependent properties. However, their use is limited by their low thermal stability against sintering, which for the system under concern takes place by cluster diffusion and coalescence (Smoluchowski ripening) and starts around 500 K. Sintering destroys cluster order, broadens the size distribution and greatly reduces the cluster number density.

Here we explore embedding of an Ir cluster superlattice on Gr/Ir(111) into a matrix of elemental carbon. With increasing deposited amount of carbon, a conformal carbon coverage of the metal clusters establishes. As evidenced by scanning tunnelling microscopy, the embedding process does not affect the order of the cluster superlattice. Most important, sintering of the clusters by Smoluchowski ripening is suppressed up to the highest investigated temperatures of 1350 K.

[1] N'Diaye, AT. et al., New Journal of Physics, 2009

O 82.2 Thu 15:15 H5

Graphene-coating of Platinum nanoparticles — •Martha Scheffler, Georgios Pantazidis, and Liv Hornekaer — Department of Physics and Astronomy, Aarhus University, Denmark

Despite the great potential that has been reported for core-shell metal-metal nanoparticles in catalytic processes and biomedical applications, similar reports on graphene-coated nanoparticles are lacking. Graphene coatings prevent nanoparticles from sintering, increase the temperature stability, and can prevent corrosive species from blocking the catalytically active sites. For some single crystal systems, graphene coatings have been shown to have beneficial effects, improving reaction efficiency.

We will present our measurements on graphene-coated Platinum nanoparticles. We synthesized Pt nanoparticles of tens of nm in diameter under UHV conditions using an HOPG support. Via chemical vapor deposition using ethylene, we produced a graphene coating on these nanoparticles that is tested on its catalytic and reactive properties. We use scanning tunneling microscopy to describe the shape and size of the nanoparticles as well as the topography of the graphene layer.

O 82.3 Thu 15:30 H5

Dehydrogenation of Liquid Organic Hydrogen Carriers on Supported Pd Model Catalysts: Carbon Incorporation under Operation Conditions — •Ralf Schuster[1], Fabian Waidhas[1], Manon Bertram[1], Henning Runge[2], Simon Geile[2], Simon Chung[2], Vedran Vonk[2], Heshmat Noei[2], Yaroslava Lykach[1], Florian Bertram[2], Andreas Stierle[2], and Jörg Libuda[1] — [1]Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg

Hydrogen and carbon, formed during the dehydrogenation and unselective decomposition of liquid organic hydrogen carriers (LOHCs) under reaction conditions, may diffuse into the bulk of the catalyst and, thus, change its activity and selectivity. We studied the influence of hydrogen and carbon on a sapphire-supported Pd nanoparticle (NP) model catalyst under reaction conditions (500 K, 1 bar) by high-energy grazing incidence X-ray diffraction. In pure H_2 at 300 K, the Pd NPs show a continuous transition from the α-PdH to β-PdH phase with increasing H_2 partial pressures, while the miscibility gap is narrowed in comparison to bulk Pd. With increasing temperature, the hydrogen uptake decreases and at 500 K, no hydride phase is formed. Surface carbon, formed by decomposition of the LOHC at 500 K, diffuses into the NP bulk. Our studies show that this formation of bulk carbon is efficiently suppressed in the presence of H_2. This highlights the importance of controlling the partial pressure of H_2 during dehydrogenation of LOHCs over Pd-based catalysts in real hydrogen release units.

O 82.4 Thu 15:45 H5

Spectroscopic Insights to Liquid Rh-Ga Alloys for Effective Propane Dehydrogenation — •Haiko Wittkämper, Narayanan Raman, Mathias Grabau, Sven Maisel, Nicola Taccardi, Jonas Debuschewitz, Tanja Bauer, Mingjian Wu, Marco Haumann, Andreas Görling, Erdmann Spiecker, Jörg Libuda, Peter Wasserscheid, Hans-Peter Steinrück, and Christian Papp — Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

We present a study of Rhodium as active metal for selective alkane dehydrogenation. It becomes a very active, selective and stable propane dehydrogenation catalyst when incorporated in a matrix of liquid gallium on oxidic support particles. The remarkable properties of this catalyst are attested to the atomic dispersion of the active transition metal in liquid gallium nano-droplets, which is indicated by temperature dependent HRTEM. The observed temperature-dependence of the selectivity of the catalyst is due to the dissolution/precipitation of Rh-rich intermetallic phases, leading to the Rh enrichment/depletion of the liquid Ga phase as is demonstrated by temperature dependent XPS studies of Rh-Ga alloy model systems. Based on ab initio molecular dynamics simulations and density functional calculations of a possible reaction site a mechanism for the system is proposed that goes in line with what we previously proposed for similar supported catalytically active liquid metal solutions such as Pt-Ga and Pd-Ga.

O 82.5 Thu 16:00 H5

Supported catalytically active liquid metal solutions: Preparation and characterization of Pd-Ga and Pt-Ga model systems on modified HOPG — •Miroslav Kettner[1], Sven Maisel[2], Corinna Stumm[1], Matthias Schwarz[1], Christian Schuschke[1], Andreas Görling[2], and Jörg Libuda[1] — [1]Physikalische Chemie II, FAU Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen, Germany — [2]Lehrstuhl für Theoretische Chemie, FAU Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen, Germany

Single atom catalysts merge attractive properties of homogeneous and heterogeneous catalysts, such as atomically defined active sites, high selectivity, and high metal utilization. Recently, the concept of supported catalytically active liquid metal solutions (SCALMS) proved effective in creating such isolated active sites by diluting an active metal in a low melting point metallic matrix. To explore the properties of such systems under surface science conditions, we have prepared model systems for Pd-Ga and Pt-Ga SCALMS by physical vapor deposition of Pd/Pt and Ga in ultrahigh vacuum onto highly oriented pyrolytic graphite (HOPG) pre-modified by Ar^+ bombardment. We investigated the growth behavior, the morphology, the surface chemistry, and the stability of Pd-Ga and Pt-Ga alloys on HOPG by combining AFM and IRAS experiments with DFT calculations. The results prove the single atom character of the active sites in Ga-rich alloys. Thus, the Ga-rich nanoalloy systems prepared on modified HOPG present a well-suited model to study the adsorption and reaction on SCALMS by surface science methods.

O 82.6 Thu 16:15 H5

Atomic oxidation of supported CoTPP films — •Jakob Hauns, Artur Böttcher, and Manfred M. Kappes — Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

Thin Co-Tetraphenylporphyrin films, CoTPP, were grown on HOPG under UHV conditions by applying the low-energy cluster beam deposition technique (LECBD, [1]). The oxidation has been performed by exposing the films kept at room temperature to a beam of nearly-thermal oxygen atoms at a constant flux. UPS based analysis of the valence band revealed a gradual quenching of the HOMO state ($E_B \sim 1.8$ eV). The oxygen conditioned evolution of all relevant CoTPP core states supported by DFT calculations of the most stable oxides enables to follow the oxidation pathways. The sublimation of the oxidized CoTPP films has been studied by monitoring the mass spectra of the volatile species during heating the sample (MSTDS, [1]). The emission of oxidized multilayers proceeds within a broad temperature interval (450-850K). It is dominated by a series of CoTPP-O_n oxides ($0 \leq n \leq 5$) which implies that an intact CoTPP is capable to adopt up to five oxygen atoms. In contrast, the sublimation of a CoTPP monolayer deposited on preoxidized HOPG gives rise to a completely different product spectrum indicating that the substrate uniquely participates in the reaction.

[1] J. Weippert, et al. J. Phys. Chem. C DOI:10.1021/acs.jpcc.8b01655

O 82.7 Thu 16:30 H5

Defect dependent adsorption of tungsten oxide clusters on rutile TiO_2 surfaces for model (photo-)catalysis — •Lars Mohrhusen, Maximilian Grebien, and Katharina Al-Shamery — Carl von Ossietzky University of Oldenburg, Institute of Chemistry, Oldenburg, Germany

Rutile TiO_2 is one of the most intensively studied materials for heterogeneous thermal and photoinduced catalysis. In earlier publications, the importance of bulk and surface defects for the chemical reactivity of small molecules such as oxygen,[1] methanol[2] or benzaldehyde[3] has been demonstrated. In temperature programmed reaction spectroscopy (TPRS) and infrared reflection-absorption spectroscopy (IRAS), different reaction pathways such as the reductive coupling, deoxygenation to hydrocarbons and partial oxidation were significantly dependent on the defect density as well as the presence of different oxygen species.

The deposition of (oxidic) cocatalysts[4,5] is a common approach to address the (photo-)catalytic performance. However, a detailed understanding is often missing. Here, we present systematic studies on rutile TiO_2 (110) under well-defined ultra-high vacuum conditions illustrating the deposition of tungsten oxide clusters to control the defect density dependent adsorption and reactivity of small molecules.

[1] E. Lira et al., J. Am. Chem. Soc. 2011, 133, 6529. [2] M. Osmić et al., J. Phys. Chem. C 2018, DOI: 10.1021/acs.jpcc.8b02953 [3] P. Clawin et al., Chem. Eur. J 2014, 25, 7665. [4] C. Pang et al., Chem. Rev. 2013, 113, 3887 [5] J. Kim et al., Catal. Today 2007, 120, 186.

O 82.8 Thu 16:45 H5

Adsorption and Interfacial Reactions of 2H-Tetraphenylporphyrin on Cobalt Oxide Thin Films — •Daniel Wechsler[1], Cynthia Fernández[2], Quratulain Tariq[1], Nataliya Tsud[3], Kevin Prince[3,4], Federico Williams[2], Hans-Peter Steinrück[1], and Ole Lytken[1] — [1]Chair of Physical Chemistry II, University Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany — [2]Department of Inorganic, Analytical and Physical Chemistry, University of Buenos Aires, Buenos Aires C1428EHA, Argentina — [3]Elettra-Sincrotrone Trieste S.C.p.A., Strada Statale 14, km 163.5, 34149 Basovizza-Trieste, Italy — [4]IOM, Strada Statale 14, km 163.5, 34149 Basovizza-Trieste, Italy

Understanding the interactions between organic molecules and metal-oxide surfaces plays an important role in many nanotechnology devices.

We have studied the adsorption and interfacial reactions of 2H-tetraphenylporphyrin (2HTPP) with synchrotron-radiation X-ray photoelectron spectroscopy on cobalt- and oxygen-terminated Co_3O_4 and CoO cobalt-oxide thin films. Already at 175 K, we find evidence for the formation of a metalated species, most likely CoTPP, on both surfaces. The degree of metalation increases with temperature on both surfaces until 575 K, at which point desorption is observed from the reducible cobalt-terminated Co3O4 oxide, while decomposition is observed on the non-reducible oxygen-terminated CoO oxide.

The project is supported by the DFG trough FOR 1878 (funCOS).

O 82.9 Thu 17:00 H5

Artificial Leaf, catalysis of oxygen evolution with the doping of hematite — •Huu Chuong Nguyễn[1], Felipe Andrés Garcés-Pineda[1], Mabel de Fez Febré[1], José Ramón Galán-Mascarós[1,2], and Núria López[1] — [1]Institute of Chemical Research of Catalonia (ICIQ), Av. Països Catalans 16, 43007 Tarragona (Spain) — [2]Catalan Institution for Research and Advanced Studies (ICREA), Passeig Lluis Companys, 23 , Barcelona 08010,Spain

A-LEAF is a project of the European Commission for developing an efficient and economically viable photoelectrocatalytic cell (PEC). The goal is to recycle CO_2 to fuel like an artificial leaf. The two most important reactions in a PEC are CO_2 reduction and oxygen evolution reaction (OER). These processes are energetically costly and but can be improved with catalysis. There are several possible strategies for optimisations. One of them is by doping a material to reduce the energy barrier and improve the kinetics. In this talk, we will present the general framework of A-LEAF, the basic concepts and theory of catalysis, Density Functional Theory, CO_2 reduction and oxygen evolution with a practical example; the doping of hematite as a model catalyst for the OER. Hematite ($\alpha-Fe_2O_3$) is a non-toxic, cheap and abundant material. Doped with redox or non-redox active species, it presents very different performances and catalytic pathways. Using both experimental and theoretical techniques, we will show how doping with non-redox and redox dopants differs, how Proton-Coupled-Electron-Transfer is involved and how this affects the global catalytic performance.

O 82.10 Thu 17:15 H5

Near-Surface Doping of Rutile RuO2 for Optimizing the Oxygen Evolution Reaction — •Manuel J. Kolb[1,2] and Frank Abild-Pedersen[1,2] — [1]SLAC National Laboratory, Stanford, USA — [2]Stanford University, Stanford, USA

The electrochemical oxygen evolution reaction plays a fundamental role in the current limitations to the efficiency and viability of hydrogen-oxygen-based fuel cells. Recent experimental and theoretical work [1,2] on the pre-oxygen-evolution region of the RuO2(110) voltammogram found evidence for the existence of stable dioxygen species, in contrast to earlier theoretical calculations [3]. Based on this new information we investigated the possibilities of doping RuO2(110) with a variety of metal dopant atoms and their influence on the adsorption energies of these oxygen-related species.

[1] R. Rao et al, Energy & Environmental Science, 2017, 10, 2626-2637 [2] K. Stoerzinger et al, ACS Energy Lett., 2017, 2(4), 879-881 [3] I. Man et al, ChemCatChem, 2011, 3, 1159-1165

O 82.11 Thu 17:30 H5

Electrical and Protonic Conductivity of Surface Modificated Porous Yttria-Stabilized Zirconia (YSZ) Thin Films — •Erdogan Celik and Matthias T. Elm — Center for Materials Research, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen

Porous yttria-stabilized zirconia (YSZ) thin films were prepared using pulsed laser deposition in order to investigate the influence of the high surface area on the electrical transport properties. Electrochemical impedance spectroscopy was carried out as a function of temperature, oxygen activity and humidity of the surrounding atmosphere. At high humidity protons on the surface of the porous YSZ thin films lead to an increased conductivity, especially at low temperatures. By coating the porous YSZ films with a titania (TiO2) film of only a few nanometers, the protonic contribution to the conductivity at low temperatures is completely suppressed revealing the large influence of the surface on the transport properties of porous materials.

O 83: Organic Molecules on Inorganic Substrates VI: Chirality, Charge Transfer, Self-Assembly

Time: Thursday 15:00–17:30 Location: H9

O 83.1 Thu 15:00 H9

Supra-molecular spirals formed by self-assembly of spiral shaped molecules — •Jan Voigt[1], Milos Baljozovic[1], Kévin Martin[2], Narcis Avarvari[2], Karl-Heinz Ernst[1], and Christian Wäckerlin[1] — [1]Empa, Dübendorf, Switzerland — [2]Université d'Angers, France

The interdependence of macroscopic and molecular chirality, which is ubiquitous in nature, is still lacking scientific insight. Here, the 2D crystallization of benzene-1,3,5-tris[4]helicene on the Ag(111) surface is studied with scanning tunneling microscopy. The molecules consist of three [4]helicene subunits, which are intrinsically chiral, attached to a central benzene ring via sigma bonds. The helical arms have a low barrier of inversion and the sigma bonds allow for additional configurational flexibility. Indeed, deposition on the sample kept at room temperature leads to self-assembled, homochiral arrays of spiral shaped trishelicenes. Above a critical coverage, mesoscopic supramolecular spirals are formed. These supramolecular arrangements occur with different topology and their handedness is determined by the chirality of the molecular spirals in the self-assembled domain.

O 83.2 Thu 15:15 H9

Two-dimensional racemate crystallization of trioxa-[11]helicene molecules on Ag(100) surface — •Bahaaeddin Irziqat[1], Shyam Sundar[2], Ashutosh Bedekar[2], and Karl-Heinz Ernst[1] — [1]Empa, Dübendorf, Switzerland — [2]University of Baroda, Vadodara, India

Intermolecular chiral recognition in two-dimensional self-assembly on metal surfaces is of paramount importance for enantiomeric separation and heterogeneous enantioselective catalysis for the production of chiral pharmaceuticals and liquid crystal devices. Two-dimensional nucleation and crystallization of a racemic mixture of the helical aromatic hydrocarbon trioxa-[11]helicene (7,12,17-trioxa[11]helicene) on the single crystalline (100) surface of silver has been studied using a combination of scanning tunneling microscopy and theoretical molecular modeling. After deposition on the surface kept at room temperature, the molecules form islands that are comprised of domains in line with the principal directions of the substrate. The domains are heterochiral, with alternating enantiomer sequence in one lattice direction and non-alternating enantiomer sequence in the other.

Invited Talk O 83.3 Thu 15:30 H9

Control of charge transfer into large organic molecules on ultrathin MgO(001) films — •Martin Sterrer — University of Graz, Graz, Austria

Charge transfer processes on ultrathin, supported oxide films have received increasing attention in recent years because of the possibility to control the charge state of adsorbates or the direction of catalytic reactions. The main driving forces for the occurence of charge transfer in these systems is the reduction of the substrate work function induced by deposition of the oxide film in combination with an adsorbate with high electron affinity. While previous studies have focused on the charging of metal atoms (e.g. Au) or small molecules (e.g. O_{2}, NO_{2}), we have recently extended these investigations to charge transfer processes into large organic molecules. In this contribution, we present results on the adsorption and charging of pentacene (5A) and tetraphenylporphyrin (2H-TPP) on ultrathin MgO(001) films supported on Ag(001). By combing scanning tunneling microscopy and photoemission spectroscopy and tomography, we are able to identify and quantify charge transfer into the organic monolayer film. In addition, we show that by variation of the work function and the MgO thickness it is possible to drive the system into a state where no charge transfer occurs. In the case of 2H-TPP charge transfer also appears to strongly influence the self metalation of 2H-TPP to Mg-TPP. Thus, our investigations lay the basis for the ultimate control of charge transfer, and the related chemistry, on ultrathin oxide film systems.

O 83.4 Thu 16:00 H9

Chirality transfer through multistep reaction processes — •Mohammed S. G. Mohammed[1,2], Nestor Merino-Díez[1,2,3], Jesus Castro-Esteban[4], James Lawrence[1,2], Alejandro Berdonces Layunta[1,2], Luciano Colazzo[1,2], Jose Ignacio Pascual[3,5], Diego Peña[4], and Dimas G. de Oteyza[1,2,5] — [1]Donostia International Physics Center (DIPC), San Sebastian, Spain — [2]Materials Physics Center, Centro de Física de Materiales (CSIC/UPV-EHU), San Sebastian, Spain — [3]CIC nanoGUNE, San Sebastián, Spain — [4]Centro de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS), Departamento de Química Orgánica, Universidade de Santiago de Compostela, Santiago de Compostela, Spain — [5]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Besides its interest for potential optoelectronic devices, molecular chirality is of utmost importance in biology and medicine. Consequently relevant is the selective synthesis of enantiopure molecular compounds, which has been hardly addressed in the growing field of on-surface synthesis. In this frame, 2,2*-dibromo-9,9*-bianthracene reactants are known to form chiral graphene nanoribbons on coinage metal substrates through a complex multi-step reaction including an initial polymerization by Ullmann coupling and following cyclodehydrogenation steps.In this work we show how, starting from enantiopure reactants deposited onto Au(111), their chirality is sequentially transferred to the polymers and finally to the GNRs with an excellent level of selectivity. Unambiguous evidence of this effect is obtained by high-resolution images of the polymers and GNRs at the single molecule level.

O 83.5 Thu 16:15 H9

Influence of Substrates on Self-Assembled Terphenyl Monolayers Investigated by NC-AFM and FM-KPFM — •Niklas Biere[1], Sascha Koch[2], Patrick Stohmann[2], Yang Yang[2], Armin Gölzhäuser[2], and Dario Anselmetti[1] — [1]Experimental Biophysics & Applied Nanoscience, University of Bielefeld, Germany — [2]Physics of Supramolecular Systems and Surfaces, University of Bielefeld, Germany

Carbon Nano Membranes (CNM) are mechanical stable and homogeneous quasi 2D systems, which are formed by electron radiation induced, cross-linked self-assembled monolayers (SAM). Contrary to graphene, the CNM structural and functional properties can be tailored by the selection of precursors for the SAM formation [1]. CNMs show the capability to act as a molecular sieve to filter e.g. water molecules from impurities with extraordinary efficiency [2]. While this result promises remarkable applications, the actual process of CNM formation as well as their structure and the mechanism for water permeation is still in the focus of our investigations. Furthermore, the choice of substrate influences the self-assembly of our precursor molecules more than previously expected, even with isoelectronic surfaces like gold and silver. In this work, we will present data acquired by noncontact AFM combined with FM-KPFM under ultra-high vacuum conditions to investigate and compare the morphology of in-situ prepared SAMs and CNMs of terphenylthiols on Au(111) and Ag(111).

[1] A. Turchanin, A. Gölzhäuser, Adv. Mater. 28 (2016) 6075-6103. [2] Y. Yang et al., ACS Nano 12 (2018) 4695-4701.

O 83.6 Thu 16:30 H9

Large thermal expansion of a self-assembling monolayer in UHV — •Sebastian Scherb[1], Antoine Hinaut[1], Guilherme Vilhena[1], Rémy Pawlak[1], Akimitsu Narita[2], Thilo Glatzel[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Max Planck Institute for Polymer Research, Mainz, Germany

Self-assemblies of structurally complex molecules in UHV provide interesting prospects for applications in optoelectronics, nanomechanical devices and molecular electronics. To investigate their viability for specific applications, high-resolution studies of their behavior under a variety of conditions are required.

In this study we report the experimental and theoretical study of the adsorption behavior of a molecular assembly on Au(111) under different thermal conditions. A shape persistent polyphenylene Spoked Wheel molecule [1] was deposited onto Au(111) surfaces in UHV by electrospray deposition [2]. The assembly formation studied at room temperature by ncAFM and at low temperature by STM/AFM shows a large positive thermal expansion coefficient from LT to RT. Comparing with molecular dynamics simulations we propose an explanation of the mechanism of expansion due to alkyl chain mobility in combination with increased molecular diffusion.

[1] Liu, Y. et al., J. Am. Chem. Soc., 138, 15539-15542 (2016). [2] Hinaut et al., Nanoscale, 10, 1337-1344 (2018).

O 83.7 Thu 16:45 H9

Structure and electronic properties of end states of self-assembled 1D covalent molecular chains on Au(111) — •Ales Cahlik[1], Jack Hellerstedt[1], Martin Svec[1], Vjai Meena Santhini[1], Simon Pascal[2], Pingo Mutombo[1], Karel Výborný[1], Olivier Siri[2], and Pavel Jelinek[1] — [1]Institute of Physics, ASCR, v.v.i., Cukrovarnická 10, CZ-16253 Praha 6, Czech Republic — [2]Aix Marseille Université, CNRS, CINaM UMR 7325, 13288, Marseille, France

1D structures offer a rich ecosystem for realizing quantum states with potential application for advanced information technologies. Surface confined molecular self-assembly is one avenue for creating 1d systems, where the extant structure is controlled by the precursor shape, and functional group interlinking chemistry. Here we study self-assembled 1d chains of zwitterionic molecule bis-bidentate ditopic (DABQDI) on Au(111) in ultrahigh vacuum, measured at 5K using combined scanning tunneling and non-contact atomic force microscopies (STM/ nc-AFM). Submolecular resolution achieved with a CO- functionalized tip offers detailed structural information, specifically regarding the unusual hydrogen bonds linking the precursor units. In-gap electronic states near the Fermi energy are observed via scanning tunneling spectroscopy (STS), strongly localized to the chain ends. We present our latest efforts to understand and simulate the observed structures via density functional theory (DFT) and nc-AFM simulations, and rationalize the observed electronic properties via modelling inspired by the Su, Schrieffer, Heeger (SSH) one-dimensional tight binding model.

O 83.8 Thu 17:00 H9

Adsorption Structure of Mono- and Diradicals on a Cu(111) Surface: Chemoselective Dehalogenation of 4-Bromo-3"-iodo-p-terphenyl — •Daniel Ebeling[1], Qigang Zhong[2], Tobias Schlöder[3], Jalmar Tschakert[1], Pascal Henkel[3], Sebastian Ahles[4], Lifeng Chi[2], Doreen Mollenhauer[3], Hermann A. Wegner[4], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, 215123 Suzhou, P. R. China — [3]Institute of Physical Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany — [4]Institute of Organic Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany

For building molecular nanostructures on surfaces the knowledge about the precise adsorption geometry of intermediates at different stages during the reaction process and their interactions with surface atoms or adatoms is of fundamental importance. We show the selective dehalogenation of 4-bromo-3"-iodo-p-terphenyl on Cu(111) using bond imaging atomic force microscopy with CO functionalized tips. The deiodination and debromination reactions are triggered either by heating or locally applying voltage pulses with the tip. In connection with first principles simulations we can determine the orientation and position of the pristine molecules as well as adsorbed mono- and diradicals and the halogens. In particular, for the radicals we observe strongly twisted and bent 3D adsorption structures.

O 83.9 Thu 17:15 H9

Complex Probe Particle Model Simulations Supporting nc-AFM Experiments — •Ondrej Krejci[1], Fabian Schulz[1,2], Juha Ritala[1], Ari P. Seitsonen[3], Peter Liljeroth[1], Shigeki Kawai[4], Remy Pawlak[5], Feng Xu[6], Lifen Peng[6], Akihiro Orita[6], Ernst Meyer[5], Tomihiko Nishiuchi[7], Keisuke Sahara[7], Takuya Kodama[7], Takashi Kubo[7], and Adam S. Foster[1,8,9] — [1]Aalto Uni., Espoo, Fin. — [2]IBM Zurich, Swi. — [3]Ecole Normale Superieure, Paris, Fra. — [4]NIMS, Tsukuba, Jap. — [5]Uni. of Basel, Swi. — [6]Okayama Uni. of Science, Okayama, Ja. — [7]Osaka Uni., Toyonaka, Jap. — [8]Kanazawa Uni., Kanazawa, Jap. — [9]Johannes Gutenberg Uni., Mainz, Ger.

I will present simulations of systems studied experimentally with a CO-tip AFM/STM and development of the probe particle AFM model. [1,2] The presentation will also contain description of the experiments and DFT calculations of the systems: The first is hBN/Ir(111). Unexpected contrast was observed in CO-tip AFM images. Complex electrostatics of the tip [3] helped us to understand the origin of the contrast. [4] The other systems are non-planar molecules adsorbed on Cu(111) and Au(111). More realistic description of the CO tip, [5] were found to be important for better agreement between simulations and experiments on these molecules. [6]

[1] Hapala et al. PRB 90, 085421, 2014. [2] Hapala et al. PRL 113, 226101, 2014. [3] Ellner et al. Nano Lett. 16, 1974, 2016. [4] Schulz et al. ACS Nano 12, 5274, 2018. [5] Di Giovannantonio et al. JACS 140, 3532, 2018. [6] Kawai et al. ACS Nano 12, 8791, 2018.

O 84: Focus Session: Spins on Surfaces II (joint session O/MA)

Time: Thursday 15:00–18:00 Location: H15

Invited Talk O 84.1 Thu 15:00 H15

Long-lived magnetic states in atomic-scale magnets — •Sebastian Stepanow — ETH Zürich, Switzerland

Magnetic atoms on surfaces are emerging as a new class of systems with exceptionally long spin relaxation times, which allows for reading and writing magnetic bits on the atomic scale. The magnetic properties of the single-ion magnets depend crucially on their atomic environment and enhancing their spin dynamics may lead to the development of single-atom qubits. Recent observations of magnetic remanence in individual Ho atoms adsorbed on ultrathin MgO(100) layers on Ag(100) provided the first evidence of a single atom magnet on a surface. The opening of the hysteresis loop indicates that the lifetime of Ho atoms is on the order of hours at cryogenic temperatures. Meanwhile more rare-earth adatom systems have been identified having exceptionally long spin relaxation time T_1. Despite the raising interest in these systems, it is still not clear which factors determine their very long relaxation time and if a long coherence time can be expected. The talk highlights our recent efforts in the understanding of the different contributing factors, i.e., the strong uniaxial magnetic anisotropy, the symmetry protection of the ground state from quantum tunneling and other first order scattering processes, and the peculiarities of the spin-phonon coupling with the supporting substrate.

O 84.2 Thu 15:30 H15

Mechanism of spin-dependent electron transfer on ferromagnetic interfaces: an ab initio study — •Simiam Ghan, Karsten Reuter, and Harald Oberhofer — Chair of Theoretical Chemistry, Technical University of Munich, Garching, Germany.

Self-assembled monolayers of organic molecules (SAMs) on surfaces show great promise in the emerging field of molecular electronics due to tunable charge transport properties, long-range 2-dimensional order and ease of manufacture. Growth of SAMs on ferromagnetic surfaces offers the additional possibility of spin-dependent transport for molecular spintronics in e.g. spin-valves and magnetic tunneling junctions. To establish design principles for such applications, a thorough understanding of (spin)charge transport mechanisms over SAM-metal interfaces is of great importance.

As an initial benchmark, we report calculations of spin-dependent electron transfer in model systems of Argon monolayers on ferromagnetic Fe(110), Co(0001) and Ni(111) substrates. Spin-polarized charge transfer rates are calculated from the Fermi Golden Rule using a Hamiltonian derived from first-principles density functional theory. A faster transfer of minority spins from Argon to substrate is predicted, in excellent agreement with experiment. The scheme allows us to compare the roles of orbital geometries (i.e. their spatial character) and couplings, versus densities of acceptor states in determining a final preferential spin transfer. The benchmarked protocol is applied to thiol-based model SAMs with an aim towards predicting tunable spin-transport behavior.

O 84.3 Thu 15:45 H15

Unraveling the Oxidation and Spin State of Mn-Corrole — •Reza Kakavandi[1], Mateusz Paszkiewicz[1], Hazem Aldahhak[2], Uwe Gerstmann[2], Wolfgang Schofberger[3], Wolf Gero Schmidt[2], Johannes V. Barth[1], and Florian Klappenberger[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]Department of Physics, Paderborn University, Germany — [3]Institute of Organic Chemistry, Johannes Kepler University, Austria

The ability of engineering oxidation states and spin configurations in metal-corroles have fueled the vision of metal complexes-based platform for faster catalysis and more efficient fuel cells. One of the challenges in the functionality of corroles is to devise ways to unveil and ultimately control the electronic structure of the metal centers. However, despite the importance in implementation this class of molecules in novel devices, their electronic structure is hardly accessible with traditional techniques and thus is still under debate, especially at the interfaces. Here, via X-ray spectroscopic investigations and density functional theory calculations we explore the electronic ground state of the prototypical Mn-5,10,15-tris(pentafluorophenyl) corrole complex within a highly pure multilayer. The theory-based interpretation of Mn photoemission and absorption fine-structure spectra (3s and 2p and L2,3-edge, respectively) evidence a Mn(III) oxidation state with an S = 2 high-spin configuration. Furthermore, we shine light on the influence of being in contact to a Ag(111) surface and discuss mechanism such as charge transfer and annealing induced chemical conversions and their impact on the spin properties.

O 84.4 Thu 16:00 H15

Magnetic excitation spectra of single atoms on magnetic and non-magnetic substrates — •Juba Bouaziz, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

At low temperatures, inelastic scanning tunneling spectroscopy is a tool of predilection for the inspection of magnetic excitation spectra of single atoms deposited on surfaces. We employ a first-principles approach for the computation of the inelastic tunneling spectra relying on the Korringa-Kohn-Rostoker Green function method in combination with time-dependent density functional theory and many-body perturbation theory [1]. We extend the method to account for non-collinear magnetism and spin-orbit driven phenomena. The central quantity of our work is the electron's self-energy which encodes the coupling of the electron to the spin-excitation and renormalizes the electronic structure. We investigate $3d$ transition metal adatoms deposited on non-magnetic substrates such as Re(0001) and on magnetic surfaces such as PdFeIr(111) capable of hosting magnetic skyrmions [2,3].
[1] B. Schweflinghaus *et al.* Physical Review B **89**, 235439 (2014).
[2] N. Romming *et al.* Science **341**, 636-639 (2013).
[3] D. M. Crum *et al.* Nature Communications **6**, 8541 (2015).
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O 84.5 Thu 16:15 H15

Anisotropic spin-split surface states in momentum space from molecular adsorption — •Rico Friedrich[1,2], Vasile Caciuc[1], Bernd Zimmermann[1], Gustav Bihlmayer[1], Nicolae Atodiresei[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Present address: Center for Materials Genomics, Duke University, Durham, NC 27708, USA

Achieving control over the surface state spin texture can open new prospects in spintronics. We have recently demonstrated from first principles that the spin texture of a surface Rashba system can be controlled by the adsorption of molecules [1].

The molecular adsorption can also be employed to modulate the surface electronic structure in different momentum space directions, creating anisotropic spin splittings in **k**-space [2]. This effect is caused by an asymmetric adsorption of the molecules. Physisorbed NH$_3$ gives rise to variations of the surface state Rashba parameters up to a factor of 1.4 over the surface Brillouin zone. In contrast, chemisorption of BH$_3$ leads to variations by more than a factor of 2.5. Consequently, the anisotropy carries over to a modulation of the surface state spin texture: the spin direction can be changed from in-plane to predominantly out-of-plane by modifying the electronic momentum by 90°.
[1] R. Friedrich, *et al.*, New J. Phys. **19**, 043017 (2017).
[2] R. Friedrich, *et al.*, Phys. Rev. B **96**, 085403 (2017).
This work was supported by the Volkswagen-Stiftung (Optically Controlled Spin Logic project) and DFG SFB 1238 (Project C01).

O 84.6 Thu 16:30 H15

Tuning the coupling of an individual magnetic impurity to a superconductor: quantum phase transition and transport — •Laëtitia Farinacci[1], Gelavizh Ahmadi[1], Gaël Reecht[1], Michael Ruby[1], Nils Bogdanoff[1], Olof Peters[1], Benjamin W. Heinrich[1], Felix von Oppen[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Germany — [2]Dahlem Center for Complex Systems, Berlin, Germany

Magnetic impurities on superconductors induce via exchange scattering local bound states, so called Yu-Shiba-Rusinov states, in their vicinity. Depending on the coupling strength between the impurity and the substrate, the system can be in a free- or screened-spin ground state.

Here, we use the flexibility of a Fe-porphin molecule on a Pb(111) surface to tune continuously and reversibly between these ground states. By approaching the STM tip toward the molecule we modify on the one hand the bound state energy and on the other hand the junction transport properties so that we can resolve the YSR excitations by single-electron as well as by (multiple) Andreev reflections. [1]

[1] Farinacci et al., PRL 121, 196803 (2018)

O 84.7 Thu 16:45 H15

Investigation of the effect of Mn adatoms on the critical current in a STM Josephson junction — •Nils Bogdanoff[1], Rika Simon[1], Olof Peters[1], Gaël Reecht[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Univ. Grenoble Alpes, Inistitut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

Atomic spins on superconducting surfaces introduce so called Yu-Shiba-Rusinov (YSR) states inside the superconducting gap as fingerprint of a magnetic interaction. Furthermore, theory predicts a renormalization of the local order parameter. Differential conductance spectroscopy reveals the YSR states but not the intrinsic order of the superconducting groundstate. Using a Josephson junction the order parameter can be determined directly by measuring its characteristic critical current. We use a Pb tip in a scanning tunneling microscope (STM) and a Pb substrate as a SIS junction. The precise control over the STM tip enables high real-space resolution to study for example defects on atomic length scales. As was shown before [1], a reduction of the critical current can be observed on iron adatoms on a Pb(110) surface.
Here, we measure the critical current caused by Mn adatoms on Pb(111) in voltage- and current-biased Josephson junctions. We show that these more strongly reduce the critical current than the Fe adatoms.
[1] M. T. Randeria et al., Scanning Josephson spectroscopy on the atomic scale, Phys. Rev. B 93, 161115(R), 2016

O 84.8 Thu 17:00 H15

Broadband noise spectroscopy of antiferromagnetic iron dimers — •Gregory McMurtrie[1,2,3], Max Hänze[1,2,3], Luigi Malavolti[1,2,3], and Sebastian Loth[1,2,3] — [1]Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Structure and Dynamics of Matter, Hamburg, Germany — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany

Spin and charge dynamics are particularly pronounced in nanoscale materials, where they give rise to exciting effects such as quantum interference or quantum critical behavior. Accessing these dynamics on their intrinsic length and time scales is an important step towards a microscopic understanding of quantum physics on the atomic scale. Applying pulses [1] or continuous wave signals [2] to individual atoms has proven a powerful technique for the characterization of fast magnetic surface dynamics using scanning tunneling microscopy. We show that the dynamics of individual atoms can be observed in the frequency domain using broadband noise detection, thereby non-invasively revealing picosecond-scale fluctuations. This method is a powerful tool for characterizing both state lifetimes and measuring surface scattering effects, giving deeper insight into the fundamental dynamic behavior of spins coupled to dissipative environments. [1] S. Loth, M. Etzkorn, C. P. Lutz, D. M. Eigler, A. J. Heinrich, Science 329 1628 (2010) [2] S. Baumann, W. Paul, T. Choi, C. P. Lutz, A. Ardavan, A. J. Heinrich, Science 350 6259 (2015)

O 84.9 Thu 17:15 H15

Ab-initio study of the electron-phonon interaction of a single Fe adatom on the MgO/Ag(100) surface — •haritz garai-marin[1,2], julen ibañez-azpiroz[3], peio g. goiricelaya[1,2], idoia g. gurtubay[1,2], and asier eiguren[1,2] — [1]Materia Kondentsatuaren Fisika saila, Euskal Herriko Unibertsitatea UPV/EHU, Bilbo, Spain — [2]Donostia International Physics Center, Donostia, Spain — [3]Centro de Física de Materiales CSIC-UPV/EHU, Donostia, Spain

Breakthrough experimental studies have recently shown that it is possible to create stable magnetic quantum states in individual adatoms [1,2]. While the role of electronic interactions on the magnetic stability has been thoroughly investigated theoretically [3], the coupling with phonons has attracted much less attention. The aim of this work is to study, via ab-initio calculations, the effect of the electron-phonon interaction (EPI) in Fe adatoms deposited on MgO/Ag(100), a benchmark system where the EPI is believed to determine to large extent its magnetic stability [2]. Here we present the calculated electronic structure and vibrational dynamics of this system, including the local vibrations of the adatom. Furthermore, we analyze the effect of the EPI on the magnetic stability via the renormalization of the electronic properties of the adatom.

[1] F. Donati *et. al.*, Science **352**, 318 (2016). F. D. Natterer *et. al.*, PRL **121**, 27201 (2018). [2] W. Paul *et. al.*, Nat. Phys. **13**, 403 (2017). [3] N. Lorente and J.-P. Gauyacq, PRL **103**, 176601 (2009). J. Fernández-Rossier, PRL **102**, 256802 (2009). J. Ibañez-Azpiroz *et. al.*, Nano Lett. **16**, 4305 (2016).

O 84.10 Thu 17:30 H15

Spin excitations in non-collinear magnetic clusters deposited on Pt(111) from TD-DFT — •Sascha Brinker, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich

Small magnetic clusters hold great promise for future information technology. The smallest stable magnetic nanostructure on a metallic surface is a Fe trimer on Pt(111) [1]. The spin stability is strongly influenced by the excitation spectrum and by relativistic effects, like e.g. the Dzyaloshinskii-Moriya-interaction [2], which is among others responsible for non-collinear magnetic ground states. In this contribution, we generalize our time-dependent density functional theory calculations already including the spin-orbit interaction [3, 4] to non-collinear magnetic structures, focusing on magnetic clusters on Pt(111). We interpret our results with a generalized Landau-Lifshitz-Gilbert equation. We pay special attention to the anisotropic and non-local contributions to the spin pumping and damping, and to their dependence on the magnetic structure.

This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (ERC Consolidator Grant No. 681405 DYNASORE).

[1] J. Hermenau *et al.*, Nat. Comm. **8**, 642 (2017)
[2] J. Hermenau, S. Brinker *et al.*, arXiv:1811.02807 (2018)
[3] M. dos Santos Dias *et al.*, Phys. Rev. B **91**, 075405 (2015)
[4] F. S. M. Guimarães *et al.*, Phys. Rev. B **96**, 144401 (2017)

O 84.11 Thu 17:45 H15

Hyperfine interaction of individual atoms on a surface — •Philip Willke[1,2,3], Yujeong Bae[1,2,3], Kai Yang[3], Jose Lado[4,5], Alejandro Ferrón[6], Taeyoung Choi[1,2], Arzhang Ardavan[7], Joaquín Fernández-Rossier[4], Andreas Heinrich[1,2], and Christopher Lutz[3] — [1]Center for Quantum Nanoscience, Seoul, Republic of Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]IBM Almaden Research Center, San Jose, USA — [4]International Iberian Nanotechnology Laboratory, Braga, Portugal — [5]ETHZ, Zurich, Switzerland — [6]Universidad Nacional del Nordeste, Corrientes, Argentina — [7]University of Oxford, Oxford, UK

The combination of electron spin resonance (ESR) with scanning tunneling microscopy (STM) enabled spin resonance on individual atoms on surfaces [1]. Making use of the increased energy resolution of ESR-STM we can resolve and control the hyperfine interaction of single atoms [2]. Using atom manipulation we find that the hyperfine interaction strongly depends on the binding configuration of the atom as well as the proximity to other magnetic atoms. This allows us to extract atom- and position-dependent information about the electronic ground state as well as properties of the nuclear spin. Moreover, we show that the populations of the nuclear spin states can be controlled by utilizing the spin-polarized tunnel current [3].

[1] S. Baumann *et al.*, Science **350** (2015). [2] P. Willke *et al.*, Science **362** (2018). [3] K. Yang, PW, *et al.*, Nature Nano (2018).

O 85: Ultrafast Electron Dynamics at Surfaces and Interfaces II: New Methods and Developments

Time: Thursday 15:00–17:30 Location: H16

O 85.1 Thu 15:00 H16

The role of the spin-orbit interaction and the exchange interaction in the ultrafast demagnetization of antiferromagnetic RE intermetallics — •S.E. Lee[1], Y.W. Windsor[1], D. Zahn[1], K. Kliemt[2], C. Krellner[2], K. Kummer[3], C. Schüssler-Langeheine[4], N. Pontius[4], D.V. Vyalikh[5,6], U. Staub[7], and L. Rettig[1] — [1]FHI, Faradayweg 4-6, 14195 Berlin, Germany — [2]Physik. Institut, Uni. Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt am Main, Germany — [3]ESRF, 71 Avenue des Martyrs, CS40220, F-38043 Grenoble Cedex 9, France — [4]BESSY II, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — [5]DIPC, 20080 San Sebastian, Spain — [6]IKERBASQUE, 48011 Bilbao, Spain — [7]SLS, 5232 Villigen PSI, Switzerland

We have investigated the ultrafast dynamics of the antiferromagnetic rare-earth intermetallics, GdTM$_2$Si$_2$ (TM = Rh, Ir) employing time-resolved resonant magnetic soft X-ray scattering, which directly probes the transient $4f$ magnetic order. Following excitation by 40 fs pulses at 1.5 eV, GdTM$_2$Si$_2$ shows ultrafast demagnetization, which can be described by two exponential functions, one on a subpicosecond timescale and the other one on a tens of picoseconds timescale. While both compounds behave qualitatively very similar, GdIr$_2$Si$_2$ demagnetizes for a given fluence slightly more but with a slower time constant than GdRh$_2$Si$_2$. By comparing these two materials we will discuss the importance of the spin-orbit interaction and the exchange interaction for the ultrafast demagnetization for these antiferromagnetic materials.

O 85.2 Thu 15:15 H16

Comparison of RABBITT and streaking delays in attosecond time-resolved photoemission at solid surfaces — •Andreas Gebauer[1,2], Sergej Neb[1,3], Walter Enns[1], Benjamin Stadtmüller[2], Martin Aeschlimann[2], and Walter Pfeiffer[1] — [1]Bielefeld University, Germany — [2]University of Kaiserslautern, Germany — [3]ETH Zürich, Switzerland

The availability of single attosecond pulses and pulse trains paved the way to study electron dynamics at solid surfaces on their natural time scale [1] by applying either the attosecond streaking spectroscopy or RABBITT approach. Both techniques allow investigating time delays in the photoemission process from different initial states in the solid.

Here, we present a theoretical comparison between such delays that can be measured either by attosecond streaking or RABBITT, respectively. The time-resolved photoemission spectra are obtained by solving the 1D time-dependent Schrödinger equation using model potentials that were recently successfully applied to explain experimental data [2]. We show a continuous transition from the RABBITT regime to the streaking regime.

The absolute delays obtained by both methods are in agreement with each other within the available accuracy for kinetic energies >10eV. However, the evaluation of RABBITT spectra that are generated by a few-cycle infrared field is hindered by subtle systematic deviations between simulated results and commonly applied model functions.

[1] A.L. Cavalieri, et al. Nature 449, 1029 (2007)
[2] F. Siek, et al., Science 357, 1274 (2017)

O 85.3 Thu 15:30 H16

Measuring spin polarization and attosecond time delay in photoemission: current possibilities and perspectives — •Mauro Fanciulli[1,2], David Bresteau[2], Jakub Schusser[1], Zakariae El Youbi[1], Olivier Heckmann[1], Christine Richter[1], Thierry Ruchon[2], and Karol Hricovini[1] — [1]LPMS, Université de Cergy-Pontoise, France — [2]LIDYL, CEA Saclay, France

The phase term of the photoemission matrix elements is related to both the Wigner time delay of the process and to the spin polarization of photoelectrons from spin-degenerate states in the presence of spin-orbit coupling. Thus it is possible to make an estimate of the photoemission time scale by measuring the spin polarization [1].

In the first part of the talk, the model [2] that allows to indirectly access attosecond (as) time delays with spin-resolved experiments will be reviewed. In the second part, current attempts to combine spin resolution with direct femtosecond (fs) and as time resolution will be presented. We have installed an angle-resolved photoemission spectroscopy setup with a 3D VLEED spin detector at the recent Attolab beamline of CEA Saclay. The beamline provides a 10 kHz IR fs laser and a XUV laser based on high-harmonic generation. This give us the unique possibility to perform spin-resolved fs pump-probe and reconstruction of as-beating by interference of two-photon transitions (RABBIT) experiments on solid targets, with the aim of studying the spin polarization of the photoelectrons at their fundamental time scale.

[1] M. Fanciulli et al., PRL 118, 067402 (2017) [2] M. Fanciulli and H. Dil, arXiv:1806.05895 (2018)

O 85.4 Thu 15:45 H16

Visualization of Charge Carrier Motion in Nanosystems by Point-projection Microscopy — •Ivana Lapšanská, Faruk Krecinic, Melanie Müller, and Ralph Ernstorfer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

The ultrafast motion of charge carriers at the nanoscale plays a crucial role in the understanding and development of new optoelectronic devices. To visualize nanoscale dynamics, we employ femtosecond point projection microscopy (fs-PPM) - a technique based on low-energy (<200 eV) electron imaging in a pump-probe configuration. Probe electrons are photo-emitted from a nanotip by a femtosecond laser pulse, and diverge towards a sample producing an enlarged image of the electrostatic environment of a nanoscale object. The sample is optically excited by a laser pulse and the induced charge motion can be visualized via the interaction of the low-energy electrons with the carrier motion-induced local electric fields. We obtain a temporal resolution of the dynamics of charge motion down to tens of femtoseconds, with a spatial resolution down to 10 nm. We demonstrate the concept of charge motion visualization for amorphous carbon nanostructures, graphene and III-V semiconductor nanowires.

O 85.5 Thu 16:00 H16

Experimental setup for time-resolved momentum microscopy — •Jasmin Fehl[1], Katerina Medjanik[2], David Janas[1], Felix Passlack[1], Stefano Ponzoni[1], Mahdi Hajlaoui[1], Giovanni Zamborlini[1], Gerd Schönhense[2], and Mirko Cinchetti[1] — [1]Experimentelle Physik VI, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, 55128 Mainz, Germany

ARPES is the most common method to map electronic bands. Recently, momentum microscopy (MM), has been introduced as a novel highly efficient way to perform ARPES in large momentum space regions [1]. In this talk, we will discuss the realization and characterization of an experimental apparatus for laser-assisted MM. The setup is based on a sub-100 fs laser system for pump-probe experiments with pump and probe beams tunable in the whole visible spectrum (photon energy range: 1.0 eV - 6.0 eV) and repetition rate tunable from single shot up to 1 MHz. The laser is coupled to a momentum microscope equipped with a time of flight analyser. This system will allow us to probe the ultrafast dynamics in low-dimensional electron systems, with particular emphasis on hybrid interfaces - so called molecular spinterfaces [2] - and on materials with non-trivial spin-texture, such as topological insulators.

[1] Medjanik, K. et al. Nature Materials 16, 61 (2017)
[2] M. Cinchetti, V. A. Dediu, and L.E. Hueso, Nature Materials 16, 507 (2017).

O 85.6 Thu 16:15 H16

Time resolved momentum microscopy on FeRh thin films, revealing ultrafast time scales for antiferro- to ferromagnetic phase transition. — •Steinn Ymir Agustsson[1], Federico Pressacco[2], Michael Heber[3], Dmytro Kutnyakhov[3], Dmitry Vasilyev[1], Jon Ander Arregi[4], Vojtech Uhlir[4], Guenter Brenner[3], Davide Curcio[5], Yves Acremann[6], Fausto Sirotti[7], Gerd Schoenhense[1], Hans-Joachim Elmers[1], Jure Demsar[1], and Wilfried Wurth[2,3] — [1]Institute of Physics, Uni. Mainz, Germany — [2]CFEL, Hamburg, Germany — [3]DESY, Hamburg, Germany — [4]CEITEC BUT, Czech Republic — [5]Aarhus University, Denmark — [6]ETH Zurich, Switzerland — [7]École Polytechnique, CNRS, France

The development of a momentum microscope for parallel electron detection, coupled to ultrafast extreme ultraviolet laser sources allows simultaneous observation of time, momentum and energy resolved photo-electrons excited by femtosecond laser pulses. In such experiments performed at the Free Electron Laser FLASH (DESY, Hamburg) we studied the electron redistribution upon laser induced phase transition between anti-ferromagnetic and ferromagnetic phases of FeRh. By optimizing the microscope and changing the settings of the electron optics, we could strongly reduce the effect of space charge with no loss of energy or time resolution. Such experimental conditions are the key to measuring the ultrafast response of excited carriers in complex quantum materials as well as in simple metals, where photo-excited electron-electron and electron-phonon thermalization dynamics are still not fully understood.

O 85.7 Thu 16:30 H16

Momentum dependent hot electron dynamics in Ag(110) — •Tobias Eul[1], Eva-Sophia Walther[1], Michael Hartelt[1], Eva Prinz[1,2], Benjamin Frisch[1], Mirko Cinchetti[3], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center Optimas, University of Kaiserslautern, Germany — [2]Graduate School MAINZ, Germany — [3]Experimentelle Physik IV, TU Dortmund University, Germany

Electron dynamics in solid state systems and at interfaces play a crucial role for the performance of nanoscale electronic and spintronic devices. Therefore, it is essential to investigate hot electrons and the corresponding energy and momentum dissipation mechanisms in such materials.

To go beyond the energy dissipation mechanisms, we combine the well-established time-resolved two-photon photoemission technique with ToF-momentum microscopy (PEEM operated in k-space mode). From our data set, we extract and analyze cross-correlation traces for different intermediate state energies at each point of the accessible momentum space, which can be directly translated into momentum dependent lifetime maps.

Here, we focused on single crystalline Ag(110), where we observe lifetime differences of several femtoseconds, which can be correlated to the character of the optical transition as well as to the excited state dynamics of the band structure. Our first results already point to a complex momentum dependent lifetime of electrons even for simple material systems.

O 85.8 Thu 16:45 H16

Excitation and decay mechanisms in the quantum-well state system Pb/Ag(111) — •Florian Haag[1,2], Tobias Eul[1], Mirko Cinchetti[3], Martin Aeschlimann[1], and Benjmain Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany — [3]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

Hetero-metallic bilayer systems have developed into a highly tunable class of materials where the electronic properties can be controlled by the interaction across the interface. However, the implementation of low dimensional materials in new nanoscale devices is limited by the comprehension of the hot carrier dynamics of such materials.

Here, we focus on the quantum-well state system of one monolayer Pb on a Ag(111) single crystal. Using light with different polarizations, we are able to identify three different states at the Pb-Ag interface with characteristic momentum dependent lifetimes. Furthermore, we performed time-resolved 2-photon momentum microscopy (tr-2PMM) measurements with a phase stabilized interferometer to obtain information about the excitation pathways and decay mechanisms at the hetero-metallic bilayer system to extend todays understanding of the electron dynamics in low dimensional systems.

O 85.9 Thu 17:00 H16

Time- and angle-resolved photoelectron spectroscopy of the three-dimensional Dirac semimetal Cd_3As_2 — •Hermann Erk[1], Petra Hein[1], Stephan Jauernik[1], Lexian Yang[2], Yulin Chen[3], Zhongkai Liu[4], Dharmalingam Prabhakaran[3], and Michael Bauer[1] — [1]IEAP, CAU Kiel, Germany — [2]Physics Department, Tsinghua University, Beijing, China — [3]Physics Department, Oxford University, United Kingdom — [4]School of Physical Science and Technology, ShanghaiTech University, China

Dirac semimetals exhibit a characteristic linear band dispersion in the vicinity of discrete points in momentum space. The most prominent examples are 2D Dirac cones in graphene and at the surfaces of topological insulators. However, cone-shaped band dispersions were proposed to exist also in 3D [1]. A material that was experimentally verified to host a pair of 3D Dirac cones is Cd_3As_2 [2].

Here, we present first results of a time- and angle-resolved photoemission study of the (112) surface of Cd_3As_2. While the band dispersion of the Dirac cone has already been subject of several studies, only little is known about the ultrafast carrier dynamics in this material. Our technique enables us to get the first momentum-resolved insights into the dynamics in the vicinity of the 3D Dirac cone initiated by the absorption of 840 nm pump pulses. The results are discussed under consideration of recent studies of Cd_3As_2 and in comparison to ultrafast dynamics observed in related materials.

[1] S. M. Young, S. Zaheer et al., Phys. Rev. Lett. 108, 140405 (2012).

[2] M. Neupane, S.-Y. Xu et al., Nat. Commun. 5, 3786 (2014).

O 85.10 Thu 17:15 H16

Time-resolved scanning electron microscope — •Simon Däster, Yves Acremann und Andreas Vaterlaus — ETH Zurich, Switzerland

We develop a time-resolved SEM by energy-analyzing secondary electrons which provides a contrast mechanism for local potentials of a sample. This way, we intent to observe integrated microwave electronic circuits in operando.

O 86: Topology and Symmetry-Protected Materials (joint session O/MA/TT)

Time: Thursday 15:00–17:45 Location: H24

O 86.1 Thu 15:00 H24

Structural and electronic characterization of thin Fe(Se,Te) films on the quaternary (Bi,Sb)Se_xTe_{1-x} 3D topological insulator — •Philipp Kagerer, Thiago R. F. Peixoto, Celso Fornari, Hendrik Bentmann, and Friedrich Reinert — Experimental Physics VII, Julius Maximilian University of Würzburg

The combination of an s-wave superconductor iron-chalcogenide and a 3D-topological insulator (TI) has become a vivid research topic in condensed matter physics due to the proposed emergence of bound Majorana zero modes at the interface under the presence of a time-reversal-breaking magnetic field [1]. Owing to its simple cubic structure and good growth properties, thin FeSeTe layers on (Bi,Sb)Se_xTe_{1-x} pose a promising platform to test this prediction.

Here we report on the epitaxial growth and characterization of thin layers of Fe(Se,Te) on a quaternary (Bi,Sb)(Se,Te) TI single-crystal. LEED and XPS experiments as well as STM and STS scans confirm the formation of a few monolayers of Fe(Se,Te) on top of the TI substrate. Using ARPES we show the arising of the FeSeTe valence bands near the Fermi level, along with the heavily n-doped band structure of the underlying TI. In addition, photon-energy-dependent and resonant measurements using synchrotron radiation allow a distinction between substrate and overlayer bands, and show indications for strong electron correlation and a Hubbard-gap in the material [2].

[1] L.Fu, C.L. Kane, Phys. Rev. Lett. 100, 096407 (2008)

[2] M.D.Watson et al., Phys. Rev. B 95, 081106(R) (2017)

O 86.2 Thu 15:15 H24

Magnetic and Electronic Structure of the proposed Antiferromagnetic Topological Insulator $MnBi_2Te_4$ — •Raphael Crespo Vidal[1], Hendrik Bentmann[1], Thiago Peixoto[1], Alexander Zeugner[2], Anna Isaeva[2], Anja Wolter[3], Bernd Büchner[3], Mikhail Otrokov[4], Evgueni Chulkov[4], and Friedrich Reinert[1] — [1]Chair for Experimental Physics VII, Universität Würzburg, Germany — [2]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Germany — [3]Leibniz-Institute for Solid State and Materials Research, Dresden, Germany — [4]Centro de Fisica de Materials, Centro Mixto, Spain

The interplay auf magnetism and topology gives rise to new topological quantum phases with broken time-reversal symmetry like the quantum anomalous Hall state.

Here we will present single-crystal measurements on the magnetic and electronic structure of $MnBi_2Te_4$ [1], a van der Waals bonded system composed of septuple layers stacked along its [0001]-axis. The layered structure results in a high accessibility for surface science methods, while its stochiometric nature leads to intrinsic magnetism without the need of free parameters like dopand concentration. By X-Ray magnetic circular dichroism, linear dichroism and bulk magnetization measurements we determine an out of plane A-type antiferromagnetic ordering below $T_N = 24\,K$. Angle-resolved photoemission spectroscopy shows a massive Dirac-like state with an energy gap of $\sim$100 meV.

[1] M. Otrokov et al., ArXiv., 1809.07389 (2018)

O 86.3 Thu 15:30 H24

XAS/XMCD study of magnetically doped $(Bi,Sb)_2Te_3$ — •Abdul-Vakhab Tcakaev, Volodymyr Zabolotnyy, Steffen Schreyeck, Karl Brunner, Charles Gould, and Vladimir Hinkov — University Würzburg, Am Hubland, 97074 Würzburg

The magnetic topological insulators Cr:$(BiSb)_2Te_3$ and V:$(BiSb)_2Te_3$ have been extensively studied as realizations of the quantum anomalous Hall (QAH) effect. While the QAH state in V-doped films is found to be significantly superior, the differences in the electronic structure and in the mechanisms of magnetic ordering for V- and Cr-doping remain under intensive debate. Here we combine x-ray absorption(XAS) and x-ray magnetic circular dichroism (XMCD) to trace element-specific contributions to the electronic and magnetic properties of these systems. We use *ab initio* density functional theory (DFT) based multiplet ligand field theory calculations (MLFT) at Cr and V $L_{2,3}$ edges for understanding and interpreting experimental results and determine local electronic and magnetic properties of these topological insulators.

O 86.4 Thu 15:45 H24

Laser-based ARPES and pressure dependent magneto-transport studies of BiSbTe3 topological insulator — •Shiv Kumar[1], Vinod Kumar Gangwar[2], Yufeng Zhang[3,4], Prashant Shahi[5], Hitoshi Takita[1], Swapnil Patil[2], Eike Fabian Schwier[1], Kenya Shimada[1], Yoshiya Uwatoko[4], and Sandip Chatterjee[2] — [1]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima City, 739-0046, Japan — [2]Dept. of Physics, Indian Institute of Technology (BHU) Varanasi 221005, India — [3]School of Physics and Key Laboratory of MEMS of the Ministry of Education, Southeast University, Nanjing 211189, China — [4]ISSP, University of

Tokyo, Kashiwa, Chiba 277-8581, Japan — [5]Dept. of Physics, D.D.U. Gorakhpur University, Gorakhpur 273009, India

In recent years, 3D topological insulators (TIs), have drawn significant attention in condensed matter physics. Many TIs are known as good thermoelectric (TE) materials. We have grown single-crystal BiSbTe3 3D TI sample and studied structural, TE as well as pressure dependent magnetotransport properties. Large positive Seebeck coefficient confirmed the p-type nature of BiSbTe3, which is consistent with Hall measurement. We have also studied the electronic band structure using Laser-based ARPES, which revealed the existence of a Dirac-cone like metallic surface state in BiSbTe3 with a Dirac Point situated exactly at the Fermi level. The large Seebeck coefficient and good TE performance at room-temperature attract great attention for the application in TE devices. Additionally, superconductivity emerges under pressure of 8 GPa with a critical temperature of ~2.5 K.

Invited Talk O 86.5 Thu 16:00 H24

Luttinger liquid in a box: electrons confined within MoS_2 mirror twin boundaries — •Wouter Jolie[1,2], Clifford Murray[1], Philipp Weiss[3], Joshua Hall[1], Fabian Portner[3], Nicolae Atodiresei[4], Arkady Krasheninnikov[5,6], Carsten Busse[1,2,7], Hannu-Pekka Komsa[6], Achim Rosch[3], and Thomas Michely[1] — [1]II. Physikalisches Institut, University of Cologne, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [3]Institute for Theoretical Physics, University of Cologne, Germany — [4]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [5]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [6]Department of Applied Physics, Aalto University, Finland — [7]Department Physik, Universität Siegen, Germany

Two- or three-dimensional metals are usually well described by weakly interacting, fermionic quasiparticles. This concept breaks down in one dimension due to strong Coulomb interactions. There, low-energy excitations are expected to be collective bosonic modes, which fractionalize into independent spin and charge density waves.

In this talk I will present how we construct a well-isolated, one-dimensional metal of finite length using mirror twin boundaries in molybdenum disulfide (MoS_2). We demonstrate how scanning tunneling spectroscopy can identify the unique fingerprints of confined, strongly interacting states, thereby providing a direct and local experimental tool to investigate spin-charge separation in real space.

O 86.6 Thu 16:30 H24

Structure and electronic properties of antimonene layers on Bi2Se3 interfaces — •Kris Holtgrewe[1], Conor Hogan[2], and Simone Sanna[1] — [1]University of Giessen, Germany — [2]CNR-ISM, Rome, Italy

Topological insulators (TI) exhibit unconventional physical effects that have attracted the interest of the scientific community, especially when coupled to trivial insulators. A topologically insulating Bi_2Se_3 substrate covered by the trivial insulator antimonene, is an ideal testbed to study the interfacial phenomena [1], and is furthermore interesting for applications such as topological pn-junctions [2].

Much research effort has been dedicated to surface preparation [3], recording of STM and ARPES images, as well as band structure calculations. However, the Sb-coverage dependent spin texture (e. g. position of Dirac states, Rashba splitting) is still not fully understood. Our work is dedicated to the theoretical investigation of the relationships between structural motifs, band structures and STM pattern. Thereby we show that including both spin-orbit coupling and van-der-Waals interaction in our density functional theory based approach is crucial for the correct modelling of the system.

[1] K. Jin et al, Phys Rev B **93**, 075308 (2016)

[2] S. Kim et al., ACS Nano **11**, 9671 (2017)

[3] R. Flammini, S. Colonna, C. Hogan, S. K. Mahatha, M. Papagno, A. Barla, P. M. Sheverdyaeva, P. Moras, Z. S. Aliev, M. B. Babanly, E. V. Chulkov, C. Carbone, and F. Ronci, Nanotechnology **29**, 065704 (2018)

Invited Talk O 86.7 Thu 16:45 H24

Quasiparticle interferences on Type I and Type II Weyl semimetal surfaces — •Hao Zheng — School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China

A Weyl semimetal is a new topological phase of matter that extends the topological classification beyond insulators, exhibits quantum anomalies, possess exotic surface Fermi arc electron states and provides the first ever realization of Weyl fermions in physics. In a Weyl semimetal, the chirality of the Weyl nodes give rise to topological charges, which can be understood as monopoles and anti-monopoles of Berry flux in momentum space. They are separated in momentum space and are connected only through the crystal boundary by an unusual topological surface state, a Fermi arc. The surface of a Weyl semimetal has been predicted to exhibit interesting tunneling and transport properties, leading to potential electronic and spintronic applications.

We employed scanning tunneling microscopy/spectroscopy to directly visualize the coherent quasiparticle interferences on both type-I and type-II Weyl semimetal surfaces. On NbP (type-I Weyl) surface, we reveal that the surface interference channels are restricted by their surface spin and/or orbit textures and discover the existence of surface Dirac cones. On $Mo_xW_{1-x}Te_2$ (type-II Weyl), the topological Fermi arc derived quantum interference is clearly discerned. Our results may pave a new way towards the future research on a Weyl fermion related surface transport phenomena and devices.

O 86.8 Thu 17:15 H24

Bulk and Surface Electronic Structure of the Weyl-Semimetals TaP and TaAs — •Tim Figgemeier[1], Chul-Hee Min[1], Phillip Eck[2], Jennifer Neu[3], Maximilian Uenzelmann[1], Domenico Di Sante[2], Theo M. Siegrist[3,4], Giorgio Sangiovanni[2], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universitaet Wuerzburg — [2]Theoretische Physik I, Universitaet Wuerzburg — [3]National High Magnetic Field Laboratory, Tallahassee, Florida — [4]College of Engineering, FAMU-FSU, Tallahassee, Florida

Tantalum Arsenide (TaAs) and Tantalum Phosphide (TaP) are prototypical Weyl-Semimetals. We examine the electronic band structure using Angle-Resolved Photoemission Spectroscopy over a broad range of excitation energies from the VUV to the Soft X-Ray regime. With this high flexibility in photon energies, we are able to analyse the entire complex band structure of TaP in detail. In particular the surface states and the bulk band structure are identified at different photon energies and compared to first principles DFT calculations. By use of linear polarized light, we disentangle the orbital character of the Fermi arcs and other electronic states in the Fermi surface along with their connection to the bulk band structure [1].

[1] Min et al., "Orbital Fingerprint of Topological Fermi Arcs in a Weyl Semimetal", arXiv:1803.03977 (2018)

O 86.9 Thu 17:30 H24

Exploring the spin-orbital texture in a Dirac heavy metal by spin-resolving momentum microscopy — •Ying-Jiun Chen[1,2], Christian Tusche[1,2], Markus Hoffmann[3], Bernd Zimmermann[3], Gustav Bihlmayer[3], Stefan Blügel[3], and Claus Michael Schneider[1,2] — [1]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Entanglement of spin and orbital degrees of freedom in strongly spin-orbit coupled materials creates exotic spin/orbital textures in momentum space such as Rashba and topological protected surface states. Dichroism in spin-polarized photoemission plays a crucial role in understanding the influence of spin-orbit coupling on the electronic wave functions. By virtue of the recent invention of the spin-resolving Momentum Microscope, the spin-detection efficiency and momentum resolution has been improved tremendously. This development makes it now possible to probe the photoelectron spin polarization as well as linear and circular dichroism in the angular distribution over the whole Brillouin zone. In addition to the d-electron-drived Dirac-type helical spin texture, we directly characterize the momentum-dependent spin-orbital entangled states on W(110) throughout the entire surface Brillouin zone by using differently polarized light. Comparison between theory and experiment provides insights into the large anisotropy of spin relaxation in the prototype Dirac heavy metal.

O 87: 2D Materials IV: Charge Density Waves and Electronic Properties

Time: Thursday 15:00–17:30 Location: H25

O 87.1 Thu 15:00 H25

The 3×3 charge density wave in quasi-freestanding monolayer 2H-TaS$_2$ — •Joshua Hall[1], Camiel van Efferen[1], Clifford Murray[1], Matthias Rolf[1], Niels Ehlen[1], Jun Li[1], Jan Berges[2], Erik van Loon[2], Tim Wehling[2], Alexander Grüneis[1], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Theoretische Physik, Bremen Center for Computational Materials Science, Universität Bremen, Germany

We report on the 3×3 charge density wave (CDW) in a quasi-freestanding monolayer of TaS$_2$, as grown by molecular beam epitaxy on graphene on Ir(111) [1]. Investigated by scanning tunnelling microscopy, the 3×3 periodicity of the CDW is visible at liquid helium temperatures, and allows analysis of spatial CDW amplitude variations and the influence of point and line defects. Performing low temperature scanning tunnelling spectroscopy (STS) reveals a decreased density of states at the Fermi energy, indicating partial gapping of the Fermi surface. In constant current STS maps, an energy dispersive standing wave pattern is found, which firstly illustrates the quasi-freestanding nature of the TaS$_2$ islands and secondly allows partial determination of the band structure, which is compared to data from angle resolved photoemission spectroscopy of the same system.

[1] Hall et al., 2D Materials **5** 025005 (2018)

O 87.2 Thu 15:15 H25

Structure determination of the commensurate charge density wave phase of 1T-TaS$_2$ — Gevin von Witte[1], Tilman Kisslinger[2], Jan-Gerrit Horstmann[1], Kai Rossnagel[3], Alexander Schneider[2], Claus Ropers[1], and •Lutz Hammer[2] — [1]IV. Phys. Inst., Univ. Göttingen — [2]Ls. f. Festkörperphysik, Univ. Erlangen-Nürnberg — [3]Inst. f. Exp. u. Angew. Physik, Univ. Kiel

The transition metal dichalcogenide 1T-TaS$_2$ consists of van-der-Waals stacked S–Ta–S trilayers with tetrahedrally coordinated Ta atoms. Depending on temperature several charge-density wave (CDW) states are observed. Here, we present a structural analysis of the low-temperature $(\sqrt{13} \times \sqrt{13})R13.9^\circ$ CDW-phase (C-phase) by quantitative LEED-IV.

From an UHV-cleaved single crystal, we collected a large total data base comprising 128 inequivalent beams which allows to determine 78 structural parameters safely (redundancy factor $\rho = 10$). The excellent fit quality achieved is expressed by a Pendry R-factor of $R_P = 0.12$.

The C-phase shows a strongly modulated superstructure with Ta atoms arranged in Star-of-David shaped clusters. LEED-IV reveals that the CDW distortion of the topmost trilayer is practically bulk-like with only tiny vertical atomic relaxations ($\leq$0.06 Å): The clusters of Ta atoms contract laterally by up to 0.25 Å and also rotate within the superstructure cell, causing respective distortions as well as heavy bucklings ($\approx$0.20 Å) in the adjacent sulphur layers. Most importantly, we find a stacking sequence of A–A–B of the three outermost trilayers, i.e., a vertical stacking of the top trilayer and a shift by two units of the basic hexagonal lattice (6.73 Å) between the 2nd and 3rd layer.

O 87.3 Thu 15:30 H25

Atomic-scale and ultrafast melting of a charge density wave — •Mohamad Abdo[1,2,3], Shaoxiang Sheng[1], Moritz Tritschler[1], Steffen rolf-Pissarczyk[2,3], Luigi Malavolti[1,2,3], Gregrory McMurtrie[1,2,3], Max Hänze[1,2,3], Jacob Burgess[4], and Sebastian Loth[1,2,3] — [1]University of Stuttgart, Stuttgart, Germany — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [4]University of Manitoba, Winnipeg, Canada

NbSe2 is a layered transition metal dichalcogenide (TMD) that features CDW phases between 33K and 7K. These phases exhibit collective modes in phase and amplitude. The CDW is disturbed by atomic defects that act as pinning centers [1-2]. Here we use a THz-coupled scanning tunneling microscope (STM) [3] to measure the picosecond dynamic response of the CDW locally at individual atomic defects. Pairs of THz pulses excite the CDW and probe the response in the sample*s density of states with a time resolution better than 200 fs. We find an efficient excitation mechanism driven by the tip-enhanced THz electric field in the STM junction. This excitation melts the CDW by an ultrafast displacement current and triggers a rich dynamical response that varies on the scale of one unit cell of the CDW.

[1] P. Soumyanarayanan, PNAS 110, 1623-1627 (2013). [2] X. Xi, et al. Nature Nanotechnology 10, 765-769 (2015) [3] T. Cocker, et al., Nature Photonics 7, 620-625 (2013).

O 87.4 Thu 15:45 H25

Using microARPES to measure the charge density wave gap of 1T-VSe$_2$ — •Alfred J. H. Jones[1,2], Jude Laverock[1], Charles J. Sayers[3], Mattia Cattelan[4], Simon J. Bending[3], Liam S. Farrar[3], Enrico Da Como[3], and Neil A. Fox[1,4] — [1]H. H. Wills Physics Laboratory, University of Bristol, UK — [2]Department of Physics and Astronomy, Aarhus University, DK — [3]Centre for Nanoscience and Nanotechnology, University of Bath, UK — [4]School of Chemistry, University of Bristol, UK

Charge density wave (CDW) order, as seen in a number of the layered two dimensional (2D) transition metal dichalcogenides (TMDCs), leads to many and varied changes to the lattice and electronic structure. Such phenomena continue to be poorly understood for a number of strongly correlated metals, including the metallic TMDCs. Within this class of TMDCs, 1T-VSe$_2$ is especially interesting due to the strong 3D character of the CDW.

Here I will report on measurements of the electronic structure of VSe$_2$ taken from a single domain of the bulk crystal using microARPES. These measurements were made using the NanoESCA, an energy filtered PEEM instrument capable of analysing the band structure of materials from regions as small as three microns. I will present the momentum and temperature dependence of the gap that opens in the spectral function of VSe$_2$, and show that the observed behaviour is in good agreement with a mean-field weak coupling description.

O 87.5 Thu 16:00 H25

Electronic properties and magnetism of sulphur-deficient VS_2 on Au(111) — Sabina Simon, Felix Förschner, Jannik Dornseiff, Julia Tesch, and •Mikhail Fonin — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Monolayers of two-dimensional transition metal dichalcogenides (TMDs) have recently received considerable scientific interest due to their unique properties making them prospective materials for novel device applications. Among a large variety of TMDs, VS$_2$ and VSe$_2$ monolayers gained specific attention as possible 2D materials with peculiar magnetic properties. The recent discovery of ferromagnetism in VSe$_2$ [1] boosted the interest in this materials even further.

In this work we discuss the structure and local electronic properties of sulphur-deficient VS$_2$ nanoribbons on Au(111). By means of low-temperature scanning tunneling microscopy we analyze the exact atomic arrangement within the VS$_2$ nanoribbons, showing stabilization of the atomic structure with every second sulphur atomic row missing in the upper layer. We observe very strong atomic level variations in the local density of states, which are discussed with respect to emergent magnetism in VS$_2$.

[1]. M. Bonilla et al., Nature Nanotechnology **13**, 289 (2018).

O 87.6 Thu 16:15 H25

Electronic structure and charge order of monolayer VSe$_2$ — Jiagui Feng[1], •Deepnarayan Biswas[1], Akhil Rajan[1], Matthew D. Watson[1], Federico Mazzola[1], Oliver J. Clarke[1], Kaycee Underwood[1], Igor Marković[1], Martin McLaren[1], Andrew Hunter[1], David M. Burn[2], Liam B. Duffy[3], Sourabh Barua[4], Geetha Balakrishnan[4], François Bertran[5], Patrick Le Fèvre[5], Timur K. Kim[2], Gerrit van der Laan[2], Thorsten Hesjedal[3], Peter Wahl[1], and Phil D. C. King[1] — [1]University of St. Andrews, UK — [2]Diamond Light Source, UK — [3]University of Oxford, UK — [4]University of Warwick, UK — [5]Synchrotron Soleil, France

The electronic states and phases of many monolayer (ML) transition metal dichalcogenides (TMDs) found to be different from its bulk properties and this evolution of electronic properties with thickness in TMDs are still a key open question. Here we show the results of our study on molecular beam epitaxy (MBE) grown ML VSe$_2$ film on bi-layer graphene/SiC. We have measured the detail band dispersion of this material using angle resolved photoelectron spectroscopy (ARPES). The low energy electron diffraction (LEED), along with the ARPES data show an enhanced charge density wave order compare to its bulk form. Our density functional theory (DFT) calculation and X-ray magnetic circular dichroism (XMCD) measurements suggests no magnetic ordering in ML VSe_2.

O 87.7 Thu 16:30 H25

Growth and properties of VS_2 nanostructures on Au(111) — •Sabina Simon, Felix Förschner, Jannik Dornseiff, Julia Tesch, and Mikhail Fonin — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Transition metal dichalcogenides present enormous scientific interest due to their diverse properties, which can be uniquely tailored by the nature of the components, number of layers or the stacking order of the crystal. Recent theoretical calculations predict an intricate magnetic behaviour for 2D monolayers of VS_2 [1,2], which depends on its structure and chemical composition, thus propelling this material into the focus of an active research.

In this work we discuss the epitaxial growth of VS_2 nanostructures (nanoislands and nanoribbons) on Au(111). By means of low-temperature scanning tunneling microscopy we investigate the influence of growth parameters upon the structure and chemical composition of the VS_2 nanostructures. Local spectroscopic measurements reveal strong variations of the electronic properties at the atomic level due to the interaction with the substrate and the presence of sulphur defects.

[1] Y. Ma *et. al.*, ACS Nano **6**, 1695 - 1701 (2012).

[2] D. Gao *et al.*, J. Mater. Chem. **1**, 5909 - 5916 (2013).

O 87.8 Thu 16:45 H25

Material Realistic Description of Coulomb Engineering in Two-dimensional Materials — •Christina Steinke[1,2], Malte Rösner[3], and Tim Wehling[1,2] — [1]Institute for Theoretical Physics, University of Bremen, Bremen, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [3]Center for Computational Quantum Physics, Flatiron Institute, New York, USA

Heterojunctions are building blocks of various applications in modern optoelectronics. Common heterojunctions rely on interfaces of different materials in order to gain the desired spatial band-gap modulations. We investigate a new type of lateral heterojunction imprinted externally into an otherwise homogeneous monolayer of a 2d material. [1,2] In 2d semiconductors the Coulomb interaction can modify band gaps on an eV scale and can be drastically manipulated by external screening. This allows to tune the local band gaps within a monolayer by laterally structured dielectric surroundings and leads to characteristics of a heterojunction in the local density of states with a spatially sharp band gap modulation. By means of material realistic models based on ab-initio calculations we study the nature and tunability of this band-gap modulation in 2d semiconductors in dependence of the chosen environment and identify optimal candidates for Coulomb engineered 2d systems.

[1] M. Rösner et al., Nano Lett. 16(4) (2016), 2322-2327

[2] A. Raja et al., Nature Communications 8 (2017), 15251

O 87.9 Thu 17:00 H25

Coulomb engineering of two-dimensional Mott insulators — •Erik van Loon[1], Malte Schüler[1], Daniel Springer[2], Jan Tomczak[2], Giorgio Sangiovanni[3], and Tim Wehling[1] — [1]Universität Bremen, Bremen, Deutschland — [2]TU Wien, Wien, Österreich — [3]Julius-Maximilians-Universität Würzburg, Würzburg, Deutschland

Substrates provide a convenient tool for manipulating two-dimensional materials. One way the substrate affects the material is via the screening of the Coulomb interaction. Here, we investigate the impact of this substrate screening on two-dimensional Mott (that is: Coulomb interaction-driven) insulators. This requires a theoretical description of the interplay of internal and external screening and correlation. We address the metal-insulator transition in the presence of substrate screening and how the size of the gap is altered.

O 87.10 Thu 17:15 H25

Ab initio study of environmental stability, reactivity and heterostructures formation in 2D materials. — •Clotilde Cucinotta — Imperial College London

I will discuss strategies and examples on how to address, from a theoretical and computational standpoint, the description of key properties and processes occurring in different layered materials of deep technological interest (BP, TiS2, MoS2). I will illustrate how progress in the understanding of exfoliation, basal plane functionalization, chemical reactivity and heterostructures formation in this new class of materials can be achieved by adopting a comprehensive and concerted approach, i.e. combining multidisciplinary competences of experimental and theoretical research.

O 88: Electronic Structure of Surfaces II

Time: Thursday 15:00–17:45 Location: H26

O 88.1 Thu 15:00 H26

Probing the Surface States in β-Bi2Pd through YSR excitations — •Javier Zaldívar[1], Carmen Rubio-Verdú[1], Rubén Ibarrondo[1], Edwin Herrera[2], Isabel Guillamón[2], Hermann Suderow[2], and José Ignacio Pascual[1,3] — [1]CIC nanoGUNE, San Sebastián, Spain — [2]Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Spain — [3]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

β-Bi2Pd in its bulk form is a topological semimetal with spin-polarized surface states which has drawn attention on the possibility of hosting spin-triplet components in the superconducting phase [1][2]. Previous works relied on quasi-particle interference for the detection of the spin-polarized surface states in the normal state [3]. In this work, we propose an alternative route based on the analysis of the periodicities of the Yu-Shiba-Rusinov (YSR) wavefunction [4]. Using this procedure we have been able to identify the spin-polarized surface states in the superconducting condensate. Our results open the possibility of studying spin-triplet components in mixed singlet and triplet systems through magnetic impurities.

1. M. Sakano et al, Nat. Commun. 6, 8595(2015) 2. J. Kačmarčík et al, Phys. Rev. B 93, 144502(2016) 3. K. Iwaya et al, Nat. Commun. 8, 976(2017) 4. B. Heinrich et al., Prog. Surf. Sci. 93, 1 (2018)

O 88.2 Thu 15:15 H26

Spin-polarized surface states of the SIC phase in Pb/Si(111) — •Christian Brand[1,2], Herbert Pfnür[1], Jan Hugo Dil[3,4], Stefan Muff[3,4], Michael C. Tringides[5], and Christoph Tegenkamp[1,6] — [1]Leibniz Universität Hannover, Germany — [2]Universität Duisburg-Essen, Germany — [3]Swiss Light Source, Villigen, Switzerland — [4]École Polytechnique Fédérale de Lausanne, Switzerland — [5]Ames Laboratory & Iowa State University, Ames, USA — [6]Technische Universität Chemnitz, Germany

Atomic monolayers (ML) of Pb/Si(111) have been found to be superconducting below $T_C \approx 1.8\,\mathrm{K}$ [1], but the mechanism behind the evolution of these 2D states is not understood yet. In the so-called striped-incommensurate (SIC) phase close to 4/3 ML stripes with local H3- or T4-centered $(\sqrt{3} \times \sqrt{3})$-reconstruction are separated by $(\sqrt{7} \times \sqrt{3})$-domain walls. Here we present STM and (SR)-ARPES measurements at low T ($> T_C$) to evaluate the influence of the spin-orbit interaction on the Pb surface states. As it turns out the local adsorption geometry and symmetry of the atomic structure play important roles for the understanding of the measured spin-polarization by SR-ARPES showing strongly spin-polarized metallic surface states [2]. The experimental results are in very good agreement with DFT calculations [3] and reveal beside a complex spin-texture at E_F large Rashba-type and Zeeman-like spin-splittings of the Pb surface states. [1] Nature Phys. **6**, 104 (2010), [2] PRB **96**, 035432 (2017), [3] PRB **94**, 075436 (2016).

O 88.3 Thu 15:30 H26

In Situ Strain Tuning of the Dirac Surface States in Bi2Se3 Films — •David Flötotto[1,2], Yang Bai[2], Yang-Hao Chan[3], Peng Chen[2], Xiaoxiong Wang[4], Cai-Zhi Xu[2], Joseph A. Hlevyack[2], Mei-Yin Chou[3], James N. Eckstein[2], and Tai-Chang Chiang[2] — [1]Center for Soft Nanoscience, University of Münster, Germany — [2]University of Illinois at Urbana-Champaign, Urbana, USA — [3]Academia Sinica, Taipei, Taiwan — [4]Nanjing University of Science and Technology, Nanjing, China

A controlled manipulation of the bulk band gap and spin-polarized Dirac surface states of topological insulators is of great fundamental importance and relevant to novel device applications. A promising pathway involves the application of strain, which alters the interatomic lattice spacing thus induces corresponding changes in the electronic band structure. By performing angle-resolved photoemission spectroscopy and X-ray diffraction measurements during in situ tensile tests of ultrathin epitaxial Bi2Se3 films on flexible substrates we demonstrate that the band structure of the prototypical topological insulator Bi2Se3 can be reversibly tuned in situ by applying extrinsic elastic strain of up to 2.1%. In accordance with our first principle calculations, the Dirac point reversibly shifts to larger binding energies with increasing tensile strain as a result of the decreasing inter quintuple-layer distance. Our study is an important step forward towards using strain as an in-situ tool for tailoring of the functional properties of topological materials and opens new routes for a momentum-resolved quantification of strain-induced band-structure changes.

O 88.4 Thu 15:45 H26

Growth and electronic properties of Fe on Nb(110) studied by STM and STS

— •Johannes Jung, Niclas Schmidt, Artem Odobesko, and Matthias Bode — Physikalisches Institut, Universität Würzburg, Am Hubland, Würzburg, Germany

Superconductivity and ferromagnetism with the underlying singlett and triplett pairing mechanisms, respectively, are often considered two antagonistic phenomena. Here we report on the investigation of the growth and the electronic properties of Fe on the Nb(110) surface, which exhibits the highest $T_c = 9.2\,\mathrm{K}$ of all elements. In the submonolayer range we observe three kinds of Fe–islands which exhibit different surface patterns. Spatially resolved data taken at the boundary between the superconductor and the ferromagnet show a narrow transition region with a width $w_{\mathrm{sc-fm}} = 1.5 \pm 0.5\,\mathrm{nm}$. On Fe monolayer islands a small but finite conductance dip with a 10-20% reduction remains visible in normalized STS data, indicating that the superconducting wave function has a non-zero probability amplitude at the tip position. We will present date on the dependence of surface superconductivity of Nb(110) on Fe coverage and discuss implications in the context of topological superconductivity and Majorana fermions.

O 88.5 Thu 16:00 H26

Determination of the superconducting gap of Ru(0001) and observation of a proximity-induced gap in 1ML Co/Ru(0001)

— •Julian Skolaut[1], Loic Mougel[1], Marie Hervé[1], Timofey Balashov[1], and Wulf Wulfhekel[1,2] — [1]Physikalisches Institut, Karlsruhe Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institut für Technologie, 76344 Eggenstein-Leopoldshafen, Germany

The proximity effect at the interface between a superconductor and a ferromagnet is of great interest since it can, in combination with specific spin textures in the ferromagnet, potentially be used as a platform to study majorana modes.

We used a scanning tunneling microscope (STM) mounted on a dilution cryostat to investigate the superconducting gap of Ru(0001) and its dependence on the temperature.

Furthermore, Cobalt islands were grown on Ru(0001) to investigate the the proximity-induced superconducting gap on the Cobalt islands. Even though significantly reduced in intensity, the gap was observed on both substrate and islands.

O 88.6 Thu 16:15 H26

Adsorption of atomic Fe-clusters on superconducting Pb

— •Carl Drechsel, Rémy Pawlak, Philipp d'Astolfo, and Ernst Meyer — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Due to their potential use as topological qubits in quantum computers, Majorana bound states (MBS) have attracted a large interest in Physics. Recent experiments at low temperature (< 5 K) have shown that iron chains grown on lead surfaces exhibit zero-bias conductance peaks at their ends [1,2,3,4], which can be interpreted as signature for a MBS [5].

Here, we investigate the internal structure and adsorption sites of small iron clusters evaporated on lead surfaces. Combining scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS) and atomic force microscopy (AFM), we characterize the structural and electronic properties at the atomic scale. This can be used as fundamentals for fabrication methods of iron chains on lead with atom-by-atom manipulation.

[1] Nadj-Perge, S. et al.; Science 346, 602 (2014) [2] Ruby, M. et al.; Phys. Rev. Lett. 115, 197-204 (2015) [3] Pawlak, R. et al.; npj Quantum Information, 16035 (2016) [4] Feldmann, B.E. et al.; Nature Physics 13, 286-291 (2017) [5] Mourik, V. et al.; Science 336, 1003 (2012)

O 88.7 Thu 16:30 H26

Electronic structure of the LaB_6 (001)-surface

— •Florian Sohn[1,2], Philipp Buchsteiner[3], Jan Voigt[3], Martin Wenderoth[3], and Peter E. Blöchl[1,2] — [1]Institut für theoretische Physik, Technische Universität Clausthal — [2]Institut für theoretische Physik, Universität Göttingen — [3]IV. Physikalisches Institut, Universität Göttingen

Lanthanum hexaboride (LaB_6) is the first compound among the rare earth hexaborides. Due to its low work function and high melting point, LaB_6 is widely used for thermionic electron emission. Recently, the LaB_6 (001)-cleavage plane has been investigated with scanning tunneling microscopy (STM) and spectroscopy (STS). Our data shows a mainly 2×1 reconstructed surface. We rationalize the constant current topographies and differential conductance spectra by simulations based on density functional theory (DFT). Our simulations of a LaB_6 (001)-surface, terminated by chains of lanthanum ions, show, that in STM measurements with positive bias voltage the *d*-orbitals of the topmost lanthanum ions are addressed. In contrast, at small negative bias voltages, a broad feature in the local density of states below the Fermi energy could be successfully resolved by both STS and DFT and is traced back to surface boron orbitals. Our study shows the necessity of surface calculations in order to understand the experimental data in detail and can be applied to various model systems.

O 88.8 Thu 16:45 H26

STM investigation of scattering phase shifts of single non-magnetic impurity atoms buried in Cu

— •Thomas Kotzott[1], Mohammed Bouhassoune[2], Henning Prüser[1], Samir Lounis[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

Impurities in nanostructures can be crucial for the functionality of the devices. Hence, scattering properties of impurity atoms in metals have been thoroughly investigated in the past by theoretical calculations and experimental measurements of the bulk. Here, we present a study to characterize the scattering phase of single, non-magnetic atoms buried in Cu by means of scanning tunneling microscopy (STM) and density functional theory. Using the electron focusing effect we visualize single Ge and Ag atoms several layers below the Cu surface. Experiments have been performed with a home-built low-temperature UHV-STM operating at 6K. Dilute alloys were grown by co-deposition of Cu and Ag or Ge, respectively, onto a clean Cu(100) surface. Ab-initio calculations and a plane-wave toy model are compared to the data.

We can extract the phase shift from the LDOS pattern above bulk impurities which is set by depth and species of the impurity. We find that the simple model of a Lorentzian scatterer is not sufficient for understanding all the characteristics on the local scale for a non-magnetic atom. This work was supported by DFG projects LO 1659/5-1 and WE 1889/8-1.

O 88.9 Thu 17:00 H26

Dielectric surface properties of $SrTiO_3$(001) surface studied by HREELS

— •Jonas Pantzer[1], Florian Schumann[1], Manuel Bibes[2], and Wolf Widdra[1,3] — [1]Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Unité mixte de physique CNRS/Thales, 91767 Palaiseau, France — [3]Max Planck Institute for Microstructure Physics, 06120 Halle, Germany

$SrTiO_3$ is often considered as one of the most surprising materials in the complex oxides family [1]. The discovery of a two-dimensional electron gas (2DEG) at interfaces of SrTiO3 with $LaAlO_3$ [2] and the bare surface of $SrTiO_3$(001) [3] represents a milestone towards exploiting such properties in oxide devices.

Here we report on high-resolution electron energy loss spectroscopy (HREELS) studies of the $SrTiO_3$(001) surface for different preparation conditions, different doping levels, and upon adsorption of aluminum. From surface phonon-polariton and surface plasmon polariton line shapes, we extract the charge carrier contribution and the full complex surface dielectric response.

[1] Yun-Yi Pai et al., Rep. Prog. Phys. 81, 036503 (2018)
[2] Ohtomo et al., Nature 427, 423-426 (2004)
[3] W. Meevasana et al., Nat. Mater. 10, 114-118 (2011)

O 88.10 Thu 17:15 H26

Controlling fundamental electronic interactions in SrTiO3 thin films by Ni and Fe doping — •Fatima Alarab[1,2], Berengar Leikert[3], Laurent Nicolai[2], Lucie Prusakova[2], Pavol Sutta[2], Ralph Claessen[3], Jan Minar[2], and Karol Hricovini[1] — [1]Cergy-Pontoise University, Neuville, France — [2]University of West Bohemia, Plzen, Czech Republic — [3]University of Würzburg, Würzburg, Germany

Strontium titanate (SrTiO3) has been a subject of intensive discussion in recent years both experimentally as well as theoretically. Strontium titanate is an insolator with a large band gap (Eg=3.2 eV), but it can become conductive by doping with transition metals or oxygen vacancies [1]. Here we report the fabrication and electronic properties of Ni doped SrTiO3 polycrystalline and crystalline films. The polycrystalline films were prepared by reactive magnetron co-sputtering in a reactive magnetron units equipped by pure STO and Ni targets with different Ni concentration. Whereas the crystalline films were grown by pulsed laser deposition (PLD). In this experimental investigation, we used high energy ARPES, core level spectroscopy and XPD to perform the electronic properties of the films as a function of doping concentration. Our experimental results were supported by ab-initio calculations using SPR-KKR's one-step model of photoemission [2,3].

[1] F. Alarab et al., AIP Conference Proceedings 1996, 020001 (2018). [2] Braun, Rep. Prog. Phys. 59, 1267-1338 (1996). [3] H. Ebert, D. Kodderitzsch and J. Minar, Rep. on Prog. in Phys. 74, 096501 (2011).

O 88.11 Thu 17:30 H26

Investigation of Micro-stress at Si/SiO2 interface using Infrared spectroscopy — •Tahereh Mohammadi Hafshejani, Franz Königer, Jonas Wohlgemuth, Zhihua Fu, Meike Königedel, Matthias Schwotzer, and Peter Thissen — Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Silicon is by far the most important semiconductor material in the microelectronic industry mostly due to the high quality of the Si/SiO2 interface. The potential use of silicon in microelectronic devices highly depends on the interface thermal properties of between (SiO2/Si). In this work, we study how the SiO2 layer changes the interfacial properties and has a direct effect on Kapitza resistance, which has not been experimentally investigated so far. Also, vibrational properties of the SiO2 thin films (the optical phonon bands) and contribution between its thickness with the amount of Si-O bonds are discussed in details using a combination of the spectrometer with a new self-made device, applying bending forces on samples and simultaneously performing IR measurements. The results of impedance measurements have shown that Kapitza resistance at SiO2/Si interface depends on both the interfacial coupling strength and thickness. Moreover, combining infrared measurements and bending forces provide a deep insight into the processes at atomic level when the samples are under different stresses, reveal their association with a thickness of SiO2 as well as interface properties.

O 89: Annual Meeting of the Surface Science Division

Time: Thursday 19:00–19:30 Location: H1

Topics: Report of the Chairman; Presentation of the Gerhard Ertl Young Investigator Award; Miscellaneous

O 90: Post-Deadline Session

Time: Thursday 19:30–20:30 Location: H1

Contributed Post-Deadline Talks

O 91: Overview Talk: Phil King

Time: Friday 9:30–10:15 Location: H15

Invited Talk O 91.1 Fri 9:30 H15

Controlling and imaging electronic structures of Quantum Materials — •Phil King — University of St Andrews, UK

In quantum materials, strong many-particle interactions can drive a host of novel states and phases to emerge. Their collective nature, however, renders understanding, let alone controlling, the behaviour of their electrons a formidable challenge. Angle-resolved photoemission, as a momentum-resolved probe of the occupied part of the single-particle spectral function, can provide enormous insight: not only on the electronic band structures of quantum materials, but also the effects of interactions, and the opening of many-body gaps in the excitation spectrum that result from these interactions. I will illustrate how this can be used to gain new insights on controlling quantum many-body states in solids and at their surfaces. Examples include engineering magnetic instabilities [1], stabilising unexpectedly large Rashba-like spin-orbit splittings [2], strain tuning of Fermi surface topology, controlling charge-ordered states in single-layer materials [3], and studying the interplay of correlated and itinerant electrons [4].

[1] Mazzola et al., PNAS in press (arXiv:1710.05392) [2] Sunko et al., Nature 549 (2017) 492 [3] Feng et al., Nano. Lett. 18 (2018) 4493 [4] Sunko et al., arXiv:1809.08972

O 92: Electronic Structure Theory

Time: Friday 10:30–12:45 Location: H5

O 92.1 Fri 10:30 H5

Defining the Correlated Subspace in Hubbard-Corrected DFT using Boys Projector Functions — •Hanna Türk, Matthias Kick, Georg Michelitsch, Karsten Reuter, and Harald Oberhofer — Technical University of Munich

Hubbard-corrected density-functional theory (DFT+U) is an effective self-interaction correction method for DFT, which gained its current popularity particularly due to its high computational efficiency compared to other correction schemes. Applications of DFT+U rest, on the one hand, on a meaningful choice of the effective correction parameter U, a topic widely discussed in literature. On the other hand, though, the performance of the DFT+U scheme also critically depends on the choice of the projector operator, which determines the states the correction is applied to. Unfortunately, this aspect has received much less attention so far, even though a wrong choice of projector can lead to highly unphysical results.

In this contribution, we present a new projector for DFT+U implemented in the electronic structure code FHI-aims. It is based on Boys localized states, which are able to represent delocalized electrons of hybridized molecules better than other projectors based e.g. on localized atomic basis functions. We test the performance of the new Boys projector on an iron porphyrin molecule and compare it to atomically localized projector functions. Thereby, we demonstrate the effects of the choice of projector functions on the accuracy of DFT+U results and discuss the system specific suitability of different projectors.

O 92.2 Fri 10:45 H5

First-Principles Study of Cation Distribution and Electron Solvation in Alkali-Metal Doped Zeolites — •Debalaya Sarker[1], Matthias Scheffler[1], and Sergey V Levchenko[1,2,3] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Skolkovo Innovation Center, Moscow, RU — [3]NUST MISIS, Moscow, RU

Zeolites are nanoporous aluminosilicates with extraframework cations M^+, M=Na, K, Cs. Additional doping of M results in M clusters inside the zeolite pores [1], making them potential basic catalysts. Despite extensive experimental efforts, the size, charge state, and stability of the clusters, and in particular how the electrons provided by the M dopants are distributed (solvated) are still debated. By varying the Si:Al ratio, M type, and doping amount, we have studied the M distributions and electron solvation in faujasite-zeolites using van der Waals corrected [2] DFT with semilocal (PBE) and hybrid (HSE06) functionals. A cluster-expansion model is trained to explore the configurational space of the M distribution at finite temperatures. We find that the amount of exact exchange α in HSE06 has no effect on geometry and relative energies. At Si:Al$\approx$2.4, for all α the solvated electrons are localized within $\sim$3 Å around the M_4^{3+} clusters formed inside smaller β cages, but for Si:Al=5 and $\alpha \lesssim 0.1$ delocalization over the unit cell occurs. Moreover, the equilibrium distribution of framework Al is found to be different for K- and Na-exchanged zeolites, affecting the M clustering in the zeolitic pores.

[1] J. A. Rabo *et al.*, Discuss. Faraday Soc. **41**, 328 (1966).
[2] A. Tkatchenko, M. Scheffler, Phys. Rev. Lett. **102**, 73005 (2009).

O 92.3 Fri 11:00 H5

All-electron FLAPW Realization of DFPT: 2nd-order Quantities and Dynamical Matrix — •Christian-Roman Gerhorst, Markus Betzinger, Daniel Aaron Klüppelberg, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The dynamical properties of atoms in the harmonic approximation are obtained by solving an eigenvalue problem of the dynamical matrix, which is related to the second-order variation of the total energy with respect to the atom displacement. We determine the dynamical matrix employing the all-electron full-potential linearized augmented planewave (FLAPW) method, as realized in the FLEUR (www.flapw.de) code, using the density functional perturbation theory (DFPT). The formulation and realization of the DFPT in the LAPW basis is a nontrivial task, as it entails a much more sophisticated formalism compared to plane-wave codes. Due to the atom-position dependence and the discontinuities at the boundaries of the domain-wise defined LAPW basis, so-called Pulay and surface terms emerge making the realization of DFPT in FLAPW a challenge. In this contribution, we start from a brief presentation of these terms within the self-consistent solution of the Sternheimer equation, which delivers all required first-order quantities for the dynamical matrix. We will put an emphasis on how to treat the second-order changes of the external potential, the second-order variations of the wavefunction, as well as the basis-induced Pulay terms in the dynamical matrix setup, and show first results.

O 92.4 Fri 11:15 H5

Exploring the Molecular Density-Density Response Function for Inter-Molecular Interactions — •Christian Dressler, Arne Scherrer, and Daniel Sebastiani — Chemistry Departement, MLU Halle-Wittenberg, 06120 Halle(Saale), Germany

The molecular density-density response function yields the linear response of the molecular electronic charge density to arbitrary external perturbations. This motivates its application to molecular dynamics simulations, where the inter-molecular interaction potentials are constantly changing. We aim to explore this application of the molecular response function to the efficient modeling of inter-molecular interactions. Our starting point is an explicit representation of the molecular density-density response function in terms of its spectral decomposition[1]. From this representation, we devise a low rank approximation that allows to separate the contributions to the electronic response density from different multipole moments of the perturbation [2, 3]. This maximally condenses the physically relevant information of the full response function required for inter-molecular interactions. For its application to molecular dynamics simulations, we further generalize this explicit representation to arbitrary molecular geometries [4].

[1] D. Lu, F. Gygi and G. Galli., Phys. Rev. Lett. 100 147601 (2008); [2] A. Scherrer and D. Sebastiani, J. Comput. Chem. 37 665 (2016); [3] P. Ahlert, A. Scherrer, C. Dreßler and D. Sebastiani, Eur. Phys. J. B, 91 94 (2018); [4] A. Scherrer, C. Dreßler, P. Ahlert and D. Sebastiani, J. Chem. Phys. 144 144111 (2016)

O 92.5 Fri 11:30 H5

Electronic and conducting properties of single molecules with N-heterocyclic carbene terminations — Enrique Montes and •Hector Vazquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

N-heterocyclic carbenes (NHCs) have been recently shown to be a feasible alternative to thiol linker groups on Au due to their remarkable thermal and chemical stability. Here we demonstrate electron transport across single NHC-bonded single molecule circuits for the first time [1].

We investigate a series of NHC-terminated molecules by means of Density-Functional Theory and Non-Equilibrium Green's Functions, in collaboration with synthesis and experiments. We study the electronic structure and electron transport properties of a series of molecules of different length on Au electrodes. Molecules synthesized with the NHC group bonded to different metal precursors (Au, Ag, Cu) showed a modulation of conductance. Calculations reveal the effect of the NHC termination on the spectral properties of the junction [2,3] and establish the strong metal-molecule electronic coupling provided by the NHC unit.

[1] E.A. Doud, M.S. Inkpen, G. Lovat, E. Montes, D.W. Paley, M.L. Steigerwald, H. Vázquez, L. Venkataraman and X. Roy, JACS 140, 8944 (2018).
[2] G. Foti and H. Vázquez, Nanotechnology 27, 125702 (2016).
[3] G. Foti and H. Vázquez, J. Phys. Chem. C 121, 1082 (2017).

O 92.6 Fri 11:45 H5

Adsorption site-selectivity in single-molecule junctions — •Enrique Montes and Hector Vazquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Prague, Czech Republic

Knowing the geometry of the metal-molecule interface is of paramount importance in single-molecule junctions as it strongly determines its electron transport properties. This is particularly true for thiol-based junctions, where conductance can change by orders of magnitude. In this work we present a series of density functional theory (DFT) conductance calculations. We demonstrate an adsorption site-selectivity technique by combining these calculations with surface enhanced Raman scattering and current-voltage characteristics [1]. We illustrate the impact of this technique on prototypical aminobenzenethiol (ABT) and benzenedithiol (BDT) molecules connected to Au electrodes. This methodology distinguishes multiple molecular adsorption sites, and uncovers the origin of conductance fluctuations, which had never been detected experimentally up to now. In the case of ABT and BDT single-molecule junctions, electrical conductance can vary by up to a factor 100, hampering the development of reproducible conductance signatures. This study unambiguously monitors changes in molecular adsorption geometry for the first time and demonstrates their significant role on junction conductance fluctuations.

[1] S. Kaneko, E. Montes, S. Suzuki, S. Fujii, T. Nishino, K. Tsukagoshi, K. Ikeda, H. Kano, H. Nakamura, H. Vázquez and M. Kiguchi, Adsorption site recognition in single molecule circuits (submitted).

O 92.7 Fri 12:00 H5

Exact exchange-correlation kernels for optical spectra — •Mike Entwistle and Rex Godby — Department of Physics, University of York, and European Theoretical Spectroscopy Facility, Heslington, York YO10 5DD, United Kingdom

Time-dependent Kohn-Sham density functional theory (TDDFT) is in principle an exact theory of excited states in many-electron systems, such as the optical absorption spectrum of molecules and solids, but its application is severely restricted by the limitations of the available approximate functionals for electron exchange and correlation - in particular the exchange correlation kernel, f_{xc}, the functional derivative of the exchange-correlation potential with respect to the electron density. To assist the construction of more powerful approximations for f_{xc}, we calculate the exact $f_{\mathrm{xc}}(x, x', \omega)$ for a number of small, prototype systems, and analyse its character, including key aspects in which it differs from the common approximations.

O 92.8 Fri 12:15 H5

Systematic construction of the low-energy effective Hamiltonian from first-principles calculations — •Pilkwang Kim, Ji Hoon Ryoo, and Cheol-Hwan Park — Department of Physics, Seoul National University, Seoul 08826, Korea

Low-energy excitations are generally of primary interest in condensed matter physics. While first-principles methods based on density functional theory are the most reliable option, the computational cost of such methods is usually higher than other methods. On the opposite end, low-energy effective Hamiltonian methods have also been widely used as they require relatively smaller basis sets and lower computational costs. In such methods, there are some parameters that can be tuned to mimic low-energy excitations while taking account of the symmetry of the system. In this presentation, we discuss our systematic approach to construct a low-energy effective Hamiltonian that describes the electronic structure obtained from first-principles calculations. We demonstrate our method by applying it to real materials of interest.

O 92.9 Fri 12:30 H5

Atomistic study of the gas hydrates using classical molecular dynamics simulations — •Laxman Kumar Kundarapu and Anoop Kishore Vatti — Manipal Institute of Technology, Manipal, Karnataka, India

Gas clathrates are found copiously in permafrost region. In natural gas reservoirs or gas processing field, hydrates are formed by the chemical combination of the water and gas (precisely methane) at temperature above the freezing point of water. Gas clathrates are crystalline solids composed of water (ice) and gas (Methane/Ethane/Propane/CO2). The most common hydrate structure i.e. sI (structure I) is investigated. These cubic structure forms a combination of polyhedral cages (water) hosting the guest molecule (methane). We performed classical molecular dynamics (MD) simulations to understand the behaviour of gas hydrates using various water models (SPC/TIP3P/TIP4P) under extreme pressure. The structural properties and accuracy of the various water models be discussed.

O 93: Plasmonics & Nanooptics VI: Near-Field Microscopy and Phenomena

Time: Friday 10:30–13:00 Location: H8

O 93.1 Fri 10:30 H8

Electron near-field circular dichroism — •Tyler Harvey, Jan-Wilke Henke, Ofer Kfir, and Claus Ropers — IV. Physical Institute: Solids and Nanostructures, University of Göttingen, Germany

Circular dichroism spectroscopy with visible light and x-rays has long been used to characterize chiral-structured materials, magnetic materials, and chiral electronic transitions. In this presentation, we demonstrate a nanometer-resolution circular dichroism technique that employs electrons to probe optical near fields. Electron near-field circular dichroism offers nanoscale insight into chirality.

Electrons can absorb or emit integer multiples of the photon energy from an optical field adjacent to a surface [1,2]. The strength of the coupling between the electron momentum and the optical field amplitude depends on the shape and optical properties of the surface. Because electron beams can be focused to sub-nanometer spots in modern electron microscopes, this interaction, called photon-induced near-field electron microscopy (PINEM) can be employed to image plasmonic modes and optical properties with nanometer spatial resolution. By illuminating a sample with left- and right-circularly polarized light and measuring the difference in coupling strength with electrons, we probe chiral optical near fields with nanometer spatial resolution. This technique may enable the investigation of chiral optical and electronic states in plasmonic nanostructures, molecules and atoms with sub-nanometer spatial resolution.

[1] B. Barwick et al., Nature 462 (2009) 902.

[2] A. Feist et al., Nature 521 (2015) 200.

O 93.2 Fri 10:45 H8

Vectorial near-field coupling — Martin Esmann[1,2], Simon F. Becker[2], Julia Witt[2], •Anke Korte[2], Abbas Chimeh[2], Jinxin Zhan[2], Jinhui Zhong[2], Ralf Vogelgesang[2], Gunther Wittstock[2], and Christoph Lienau[2] — [1]CNRS Centre de Nanosciences et de Nanotechnologies (C2N), 91220 Palaiseau, France — [2]Carl von Ossietzky University, 26111 Oldenburg, Germany

The coherent exchange of optical near-fields between neighboring dipoles is essential for the optical properties, quantum dynamics and thus for the function of many naturally occurring and artificial nanosystems[1,2]. These interactions are inherently nanometer-ranged and depend sensitively on relative orientation, spectral detuning and dephasing, i.e., on the vectorial properties of the coupled dipolar near-fields. This makes them challenging to analyze experimentally.

Here, we introduce plasmonic nanofocusing[3] spectroscopy to record coherent light scattering spectra with 5-nm spatial resolution[4] from a small dipole antenna, excited solely by evanescent fields and coupled to plasmon resonances in a single gold nanorod. We resolve mode couplings, resonance shifts and Purcell effects as a function of dipole alignment, and show how they arise from different vectorial components of the interacting near-fields. Our results pave the way to control optical properties and function of nanoscale systems by dipolar alignment.

[1] Zhang, Y. et al., Nature 531, 623 (2016).

[2] Scholes, G.D., et al., Nature Chemistry 3, 763 (2011).

[3] Stockman, M.I., PRL 93, 137404 (2004).

[4] Esmann, M., et al., arXiv:1801.10426 (2018).

O 93.3 Fri 11:00 H8

Anisotropic scattering from gold SNOM tips and its role in the near-field light scattering spectroscopy of single nanoparticles — •Abbas Chimeh[1], Anke Korte[1], Jinxin Zhan[1], Jinhui Zhong[1], Martin Esmann[2], Nahid Talebi[3], and Christoph Lienau[1] — [1]Universität Oldenburg — [2]Centre de Nanosciences et de Nanotechnologies, Paris — [3]Max-Planck Institute for Solid State Research, Stuttgart

Plasmonic nanofocusing of light using sharp conical gold tapers enables broadband coherent spectroscopy of optical near-fields around single nanoobjects with unprecedented spatial resolution . Such measurements probe how the coupling between optical near fields of tip and sample affects the light scattering spectra from the nanofocusing gold tip. Interestingly, they reveal a coupling of the sample near-fields to both longitudinal and transversal plasmonic resonances of the tip[1], allowing to unveil the vectorial nature of the near-field coupling. To understand these couplings, knowledge about the transverse resonance, corresponding to charge oscillations perpendicular to the tip axis, are needed. Here, we employed evanescent fields at a prism surface to isolate the transverse tip resonance. By polarization resolved scattering measurements, we proved the anisotropic scattering from the tip apex comprising a longitudinal broadband dipole resonance at ~800 nm and a transversal narrowband resonance at ~550 nm. This leads to a more realistic model of tip-sample coupling proposes a novel technique for broadband near-field spectroscopy in the visible spectral range.

[1] M. Esmann et al., arXiv:1801.10426 (2018).

O 93.4 Fri 11:15 H8

Polarization in scattering near-field optical microscopy at resonant excitation — •Hamed Aminpour[1], Susanne Kehr[1], Michael Klopf[2], and Lukas Eng[1] — [1]Technische Universität Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany

Scattering-type near-field optical microscopy (s-SNOM) is a promising technique that allows to obtain optical information of samples on the nanometer length scale. Specifically, the response of molecular vibrations, phonons, and excitons in s-SNOM is particularly sensitive to the polarization direction of the incident optical field. To date, most published works focus on out-of-plane polarized s-SNOM at non-resonant excitation, only. Recently, however, excitation and detection of both in- and out-of-plane polarized local fields was demonstrated, by breaking the axial symmetry of the near-field probe [1].

In this presentation, we investigate an elegant alternative in order to achieve in-plane polarized resonant sample excitation of mid-infrared phonon modes [2]. To backup our experiments, we report here on a COMSOL simulation of the scattered near field, investigated by varying the following parameters: Angle and polarization direction of the incident light; tip-sample distance; sample permittivity as a function of wavelength. We compare these results with polarization-dependent s-SNOM measurements on $SrTiO_3$ in the spectral range from 13 to 16 μm, demonstrating the large potential of polarization-sensitive s-SNOM for the nanoscopic material analysis.

[1] K.-D. Park et al., Nano Lett. 18, 2912(2018)

[2] S. C. Kehr et al., Synchrotron Rad. News 30, 31(2017)

O 93.5 Fri 11:30 H8

Polarization-dependent resonant near-field spectroscopy in the mid- to far-infrared regime — •Lukas Wehmeier[1], Tobias Nörenberg[1], Denny Lang[2], Susanne C. Kehr[1], and Lukas M. Eng[1] — [1]Technische Universität Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany

Resonant infrared (IR) near-field spectroscopy provides a highly material-specific response with sub-wavelength spatial resolution of ∼10 nm. Here, we provide the infrared near-field response of selected paraelectric and ferroelectric materials (i.e. $SrTiO_3$, $LiNbO_3$, and $BiFeO_3$) that we investigated via scattering scanning near-field optical microscopy (s-SNOM), using the mid- to far-infrared free-electron laser (FEL) at HZDR. For these materials, we demonstrate that resonant near-field excitation is possible for both s- and p-polarized incident IR beams, which is particularly interesting for the nanoscopic investigation of anisotropic materials. We explored, for instance, the different near-field resonances of $BiFeO_3$, finding characteristic s-SNOM enhancement for three consecutive phonon modes in the 10 to 60 μm wavelength range. Utilizing the same material, we present the first realization of a superlens within the so-called THz gap, demonstrating a fascinating application of sub-wavelength imaging capabilities.

O 93.6 Fri 11:45 H8

Comparison of two approaches to near field spectroscopy on a Sb2S3 film — •Jinxin Zhan[1], Jens Brauer[1], Wei Wang[2], Lukas Schmidt-Mende[2], Petra Gross[1], and Christoph Lienau[1] — [1]Ammerländer Heerstr. 114-118, Oldenburg — [2]Universitätsstr. 10, 78457 Konstanz

Fundamental understanding of structure and function of nanomaterials is of great significance for investigating their optical and electric properties, and for further applications in corresponding fields. Optical spectroscopy on a nanometer length scale is one promising approach to obtain such insights. Here we employ scattering-type near-field scanning optical microscopy (NSOM) to probe the local spectrum of a Sb2S3 film, a very promising candidate for solar cell applications due to its high absorption coefficient and suitable bandgap. In our NSOM setup, the near field gold probe, is modulated with a frequency of 27 kHz to suppress background by demodulating the scattered optical signal at the second or third order harmonics. We measure the near field spectrum by two approaches. First, the tip is excited by a broadband pulse laser and the scattered light is recorded by a monochromator and a fast camera with up to 210 kHz line readout. Alternatively, Fourier transform spectroscopy combined with a lock-in amplifier is employed. We perform a comprehensive comparison between two methods and discuss the local spectrum information drawn from the near field spectra.

O 93.7 Fri 12:00 H8

Revisiting the Dipole Model for a Thermal Infrared Near-Field Spectroscope — •Florian Herz[1], Zhenghua An[2], Susumu Komiyama[3], and Svend-Age Biehs[1] — [1]Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany — [2]State Key Laboratory of Surface Physics and Key Laboratory of Micro and Nano Photonics Structures (Ministry of Education), Department of Physics, Fudan University, Shanghai 200433, Peoples Republic of China — [3]Department of Basic Science, The University of Tokyo, Komaba 3-8-1, Meguro-ku, Tokyo 153-8902, Japan

I will present our work on determining the scattered near-field and directly emitted power of a heated spherical nanoparticle above a sample within the framework of fluctuational electrodynamics using the dipole approximation. Additionally, for a configuration of a nanoparticle heated with respect to its environment, I show that the scattered power of the near field of the sample is strictly zero. Hence, applied on the interpretation of near-field imaging setups like thermal infrared near-field spectroscopy not only the scattering of the near field but also the direct emission of the tip has to be considered.

Reference: Florian Herz, Zhenghua An, Susumu Komiyama, and Svend-Age Biehs: Revisiting the Dipole Model for a Thermal Infrared Near-Field Spectroscope, in Phys. Rev. Applied 10, 044051 (2018).

O 93.8 Fri 12:15 H8

Hyperspectral nano-imaging applied to s-SNOM enabled by compressed sensing — •Georg Ulrich[1], Bernd Kästner[1], Franko Schmähling[1], Andrea Hornemann[1], Arne Hoehl[1], Mattias Kruskopf[1], Klaus Pierz[1], Markus B. Raschke[2], Gerd Wübbeler[1], and Clemens Elster[1] — [1]Physikalisch-Technische Bundesanstalt, Braunschweig and Berlin, Germany — [2]Department of Physics, Department of Chemistry, and JILA, University of Colorado, Boulder, 80309, USA

Scattering-type scanning near-field optical microscopy (s-SNOM) enables to circumvent the diffraction limit known from classical optics. Ultra-broadband synchrotron radiation from the Metrology Light Source (MLS) provides infrared-radiation suited for performing nano-FTIR spectroscopy [1]. However, for many applications such as mapping of biological samples hyperspectral imaging is required, resulting in a large number of spectra and therefore long acquisition time. Here we will present results from applying compressed-sensing, providing both rapid and sensitive spatio-chemical nano-imaging [2]. By reducing the number of sampling points to $1/9^{th}$ we are on the route for further enhancing the compression rate to record large data cubes. [1] P. Hermann, et al., Opt. Express. 22, 17948 (2014) [2] B. Kästner, et al., Opt. Express. 26, 18115 (2018)

O 93.9 Fri 12:30 H8

Near-Field Spectroscopy of Nanoscale Molecular Aggregates — Xing Gao and •Alex Eisfeld — MPI-PKS Dresden

When molecules are assembled into an aggregate, their mutual dipole-dipole interaction leads to electronic eigenstates that are coherently delocalized over many molecules. Knowledge about these states is important to understand the optical and transfer properties of the aggregates. Optical spectroscopy, in principle, allows one to infer information on these eigenstates and about the interactions between the molecules. However, traditional optical techniques using an electromagnetic field which is uniform over the relevant size of the aggregate cannot access most of the excited states because of selection rules.

We demonstrate that by using localized fields one can obtain information about these otherwise inaccessible states. As an example, we discuss in detail the case of local excitation via radiation from the apex of a metallic tip, which allows also scanning across the aggregate.The resulting spatially resolved spectra provide extensive information on the eigenenergies and wave functions.

[1] J. Phys. Chem. Lett. 9, 6003 (2018)

O 93.10 Fri 12:45 H8

Limitations of the kinetic theory to describe the near-field heat exchanges in many-body systems — •Christoph

Kathmann[1], Riccardo Messina[2], Philippe Ben-Abdallah[2], and Svend-Age Biehs[1] — [1]Institut für Physik, Carl von Ossietzky Universität, Oldenburg, Deutschland — [2]Institut d'Optique, CNRS, Université Paris-Saclay, Palaiseau, Frankreich

Kinetic theory based on solving Boltzmann equation is widely used to calculate heat fluxes in complex many-body systems on the nanoscale[1]. We compare this approach to an exact Landauer approach based on fluctuating electrodynamics[2] for a simple many-body system, namely a onedimensional chain consisting of nanoparticles. We find that the kinetic approach generally fails to predict heat fluxes in such a system, for polar nanoparticles we observe poor spectral agreement and a different scaling with the distance between the particles while for metallic nanoparticles the kinetic approach completely fails[3]. References: [1] J. Ordonez-Miranda, L. Tranchant, S. Gluchko, und S. Volz, Energy transport of surface phonon polaritons propagating along a chain of spheroidal nanoparticles, Phys. Rev. B 92, 115409 (2015). [2] R. Messina, M. Tschikin, S.-A. Biehs, und P. Ben-Abdallah, Fluctuation-electrodynamic theory and dynamics of heat transfer in systems of multiple dipoles, Phys. Rev. B 88, 104307 (2013). [3] C. Kathmann, R. Messina, P. Ben-Abdallah, S.-A. Biehs, Limitations of kinetic theory to describe near-field heat exchanges in many-body systems, Phys. Rev. B 98, 115434 (2018).

O 94: 2D Materials V: Novel Systems

Time: Friday 10:30–12:30 Location: H9

O 94.1 Fri 10:30 H9

Orbital texture in the band structure of a new binary honeycomb lattice AgTe — •Maximilian Ünzelmann[1], Hendrik Bentmann[1], Tilman Kisslinger[2], Lutz Hammer[2], M. Alexander Schneider[2], Thomas Fauster[2], Philipp Eck[3], Domenico Di Sante[3], Giorgio Sangiovanni[3], and Friedrich Reinert[1] — [1]Experimentelle Physik 7, Universität Würzburg — [2]Lst. f. Festkörperphysik, Universität Erlangen-Nürnberg — [3]Theoretische Physik 1, Universität Würzburg

In recent years two-dimensional (2D) materials like honeycomb-structured thin films or transition metal dichalcogenides attracted a lot of attention in solid state physics. Lattice symmetry as well as strong spin-orbit coupling leads to phenomena like non-trivial band topology (1,2). Therefore it is important to gain knowledge about the orbital character of the involved valance-state wave functions.

Here we will present a new binary honeycomb lattice namely AgTe, whose structure is realized on a Ag(111)-substrate. Using angle-resolved photoemission we will determine the 2D band structure of the AgTe layer. By means of light-polarization dependent measurements, anisotropies in the band dispersion and linear dichroism we analyze the orbital character of the valence bands. Based on the determined orbital symmetry we discuss a possible topological band inversion in AgTe.

(1) F. Reis et al., Science 357, 287 (2017)
(2) S. Tang et al., Nature Physics 13, 683 (2017)

O 94.2 Fri 10:45 H9

Stabilizing Plumbene on Fe/Ir(111): a combined experimental and theoretical study — •Gustav Bihlmayer[1], Jonas Sassmannshausen[2], André Kubetzka[2], Kirsten von Bergmann[2], Roland Wiesendanger[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Department of Physics, University of Hamburg, D-20355 Hamburg, Germany

As a heavy analog of graphene, plumbene is a two-dimensional material with strong spin-orbit effects. Although not a topological insulator, in external fields plumbene can realize a promising platform for topological phenomena [1]. Therefore, the synthesis of Pb monolayers with honeycomb structure is of substantial interest. On hexagonal substrates like Ir(111) a c(2x4) structure is found like in the graphene intercalated films on Ir [2]. In contrast, scanning tunneling microscopy images show that on a Fe covered Ir(111) surface Pb forms a honeycomb lattice. We use density functional theory calculations to rationalize these findings and analyse the impact of the hybridization on the plumbene band structure. In the unoccupied states the splitting of the Dirac cone by spin-orbit interaction is clearly observed and the influence of the iron's exchange field as function of magnetization direction is studied. In the occupied states of the freestanding plumbene we find a band inversion that leads to a topologically non-trivial gap, which undergoes strong hybridization with the substrate states.
[1] X.-L. Yu et al., Phys. Rev. B **95**, 125113 (2017).
[2] F. Calleja et al., Nature Phys. **11**, 43 (2015).

O 94.3 Fri 11:00 H9

Atomic buckling, structure and defects in silicene determined by atomic force microscopy — •Pawlak Rémy[1], Carl Drechsel[1], Philipp D'Astolfo[1], Ernst Meyer[1], and Jorge Iriba Cerda[2] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, Basel, CH 4056 — [2]Theory of Surfaces, Interfaces and Nanostructures Group, Department Nanostructures and Surfaces, Instituto de Ciencia de Materiales de Madrid, Sor Juana Inés de la Cruz, 3 28049 Madrid, Spain

The atomic buckling in two-dimensional "X-enes" [1] (such as graphene and silicene) can foster a plethora of exotic electronic properties such a quantum spin hall effect, that could be readily engineered by external strain. Quantifying buckling with sub-Å precision is however challenging, since epitaxially grown 2D-layers exhibits complex restructuring and coexist at surfaces. Here, we accurately characterize the structure, defects and atomic buckling within 0.1 Å precision of all silicene phases grown on Ag(111) using low temperature atomic force microscopy (AFM) with CO-terminated tips assisted by density functional theory (DFT). While no sign of Dirac cones is found due to the strong Ag-Si hybridization, the intrinsic buckling, varying from 0.8 to 1.1 Å, yields to slight differences in the silicene electronic properties. We think that our method pave the way for future atomic scale analysis of the interplay between structural and electronic properties in other emerging 2D-Xenes.

[1] Molle, A.et al. Nature Mat. 16, 163-169 (2017).

O 94.4 Fri 11:15 H9

Investigation of two-dimensional germanium on Ag(110) by means of XPS — •Lukas Kesper[1,2], Peter Roese[1,2], Karim Shamout[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Straße 4a, D-44221 Dortmund — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Straße 2, D-44221 Dortmund

Since the discovery of graphene in 2004 the new field of two-dimensional materials in solid state physics expanded massively. Apart from graphene other Dirac materials, like silicene and germanene, for instance, provide similar properties in a two dimensional structure [1]. Because of their strong spin-orbit coupling and tunable band gap they are predestined for realising topological field effect transistor [2]. After the report of the first synthesis of silicene [3], one dimensional silicon nano-ribbons [4] on different substrates, we present two-dimensional germanium, epitaxially grown on a Ag(110) surface. The stronger buckling and spin-orbit coupling of germanene may allow to observe the quantum spin Hall effect [2, 5]. The structural investigation of the system Ge/Ag(110) was done by using Low Energy Electron Diffraction and X-Ray Photoelectron Spectroscopy at the U55 beamline 11 at DELTA.

[1] M. Ezawa et al., Riv. Nuovo Cimento 41, 175 (2018). [2] A. Molle et al., Nature Mat. 16, 163 (2017). [3] P. Vogt et al., PRL 108, 155501 (2012). [4] C. Léandri et al., Surf. Sci. 574, L9 (2005). [5] C.-C. Liu et al., PRL 107, 076802 (2011).

O 94.5 Fri 11:30 H9

Band Renormalization of Blue Phosphorus on Au(111) — •Evangelos Golias[1,2], Maxim Krivenkov[1], Andrei Varykhalov[1], Jaime Sànchez-Barriga[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein Straße 15, 12489 Berlin, Germany — [2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Most recently, theoretical calculations predicted the stability of a two-dimensional honeycomb lattice of phosphorus atoms named blue phosphorus. We report on the successful growth of blue phosphorus on Au(111) surface using molecular beam epitaxy. We studied in detail the structural properties of blue phosphorus using low-energy electron diffraction, scanning tunneling microscopy and density functional theory calculations. Furthermore, by employing angle-resolved photoemission spectroscopy measurements we mapped the electronic structure of this novel two-dimensional allotrope of phosphorus. We find that the substrate breaks the sublattice symmetry of blue phosphorus leading to an orbital-dependent band renormalization upon the formation of a (4 × 4) superstructure on Au(111). Most importantly, the semiconducting two-dimensional phosphorus realizes its valence band maximum at 0.9 eV binding energy, however, shifted in momentum space due to the substrate-blue phosphorus interaction.

O 94.6 Fri 11:45 H9

Electrostatic Screening at the Surface of Black Phosphorus — •Brian Kiraly, Elze Knol, Daniel Wegner, and Alexander Khajetoorians — Radboud University, The Netherlands

Under applied electric fields, black phosphorus theoretically demonstrates an electronic phase transition from insulating to metallic [1]. Using chemical dopants with very small electronegativity, bulk black phosphorus can be doped into such a transition [2]; however, atomic-scale insight into the local screening and surface charge inhomogeneity is missing. Here, we probe the spatial distribution of deposited potassium adatoms on the surface of black phosphorus, with low temperature scanning tunneling microscopy, as a function of temperature and coverage. We relate the spatial distribution of adatoms to the underlying screened electrostatic potential, utilizing thermodynamic formalism, and extract the 2D vector mean potential. The data reveal the presence of extremely anisotropic, long-range interactions with strong oscillations along the zig-zag direction. The data is discussed within the context of screened Coulomb interactions, free carrier mediated Friedel-like oscillations, and strong electrostatic confinement.

[1] Q. Liu, X. Zhang, L. B. Abdalla, A. Fazzio, A. Zunger. Nano Lett. 15 (2), 2015. [2] J. Kim, S. S. Baik, S. H. Ryu, Y. Sohn, S. Park, B. G. Park, J. Denlinger, Y. Yi, H. J. Choi, K. S. Kim. Science 349 (6249), 2015.

O 94.7 Fri 12:00 H9

Calculating critical temperatures for magnetic order in 2D materials. Renormalized spin-waves vs Monte Carlo simulations — Daniele Torelli and •Thomas Olsen — Technical University of Denmark, Copenhagen, Denmark

Magnetic order in two-dimensional (2D) materials is intimately coupled to magnetic anisotropy (MA) since the Mermin-Wagner theorem implies that rotational symmetry cannot be spontaneously broken at finite temperatures in 2D. Large MA thus comprises a key ingredient in the search for magnetic 2D materials that retains the magnetic order above room temperature. Magnetic interactions are typically modeled in terms of Heisenberg models and the temperature dependence on magnetic properties can be obtained with the Random Phase Approximation (RPA), which treats magnon interactions at the mean-field level. In the present work we show that large MA gives rise to strong magnon-magnon interactions that leads to a drastic failure of the RPA. We then demonstrate that classical Monte Carlo (MC) simulations correctly describe the critical temperatures in the large MA limit and agree with RPA when the MA becomes small. A fit of the MC results leads to a simple expression for the critical temperatures as a function of MA and exchange coupling constants, which significantly simplifies the theoretical search for new 2D magnetic materials with high critical temperatures. The expression is tested on a monolayer of CrI<sub>3</sub>, which were recently observed to exhibit ferromagnetic order below 45 K and we find excellent agreement with the experimental value.

O 94.8 Fri 12:15 H9

Theoretical investigation on the magnetic properties of atomically-thin NiPS$_3$ — •Tae Yun Kim and Cheol-Hwan Park — Department of Physics, Seoul National University, Seoul 08826, Korea

Since the discovery of ferromagnetism in atomically-thin crystals [1, 2], the so-called magnetic van der Waals (vdW) materials have attracted much attention from the community of condensed-matter scientists [3]. Transition metal phosphorus trisulfide (TMPS$_3$) family is a group of antiferromagnetic vdW materials with very interesting characters. A recent Raman experiment on FePS$_3$ showed the existence of (Ising-type) antiferromagnetic order in a real two-dimensional crystal [4]. In this presentation, we will focus on NiPS$_3$, which exhibits quite different magnetic properties compared to FePS$_3$. We discuss the magnetic properties of atomically-thin NiPS$_3$ based on our recent first-principles density-functional-theory calculations on the electronic and vibrational properties and compare our results with recent experiments.

[1] B. Huang, G. Clark, E. Navarro-Moratalla, D. R. Klein, R. Cheng, K. L. Seyler, D. Zhong, E. Schmidgall, M. A. McGuire, D. H. Cobden, W. Yao, D. Xiao, P. Jarillo-Herrero, and X. Xu, Nature 546, 270-273 (2017) [2] C. Gong, L. Li, Z. Li, H. Ji, A. Stern, Y. Xia, T. Cao, W. Bao, C. Wang, Y. Wang, Z. Q. Qiu, R. J. Cava, S. G. Louie, J. Xia, and X. Zhang, Nature 546, 265-269 (2017) [3] K. S. Burch, D. Mandrus, and J.-G. Park, Nature 563, 47-52 (2018) [4] J.-U. Lee, S. Lee, J. H. Ryoo, S. Kang, T. Y. Kim, P. Kim, C.-H. Park, J.-G. Park, and H. Cheong, Nano Lett., 16 7433-7438 (2016)

O 95: Semiconductor Substrates: Metallic Nanowires

Time: Friday 10:30–13:00 Location: H14

O 95.1 Fri 10:30 H14

Novel electronic junctions in an atomic wire array: interfaces between metallic and charge density wave ordered electronic phases — •Samad Razzaq[1], Sun Kyu Song[2], Han Woong Yeom[3], and Stefan Wippermann[4] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf,Germany — [2]Center for Artificial Low D Electronic Systems, Pohang, S.Korea — [3]Center for Artificial Low D Electronic Systems, Pohang, S.Korea — [4]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf,Germany

The Si(111)-(4x1)In atomic wire array is an extremely popular model for one-dimensional electronic systems. It features a reversible, temperature-induced metal insulator transition into a charge density wave (CDW) ordered ground state with (8x2) translational symmetry. Close to the phase transition temperature, both phases can coexist and form novel types of electronic junctions between the metallic (4x1) phase and the insulating CDW-ordered (8x2) phase. Combining scanning tunneling microscopy/spectroscopy (STM/STS) and ab initio molecular dynamics calculations, we explore the microscopic structure of interfaces between distinct electronic phases at the atomic scale. Specific defects allow to modify and control the structure of these electronic interfaces. We explain the atomistic mechanism behind the junction formation and its tunability from first principles. Financial support from the German Research Foundation (DFG), grant no. FOR1700 is gratefully acknowledged.

O 95.2 Fri 10:45 H14

Coherent control of the structural phase transition in In-nanowires on Si(111) — •Jan Gerrit Horstmann, Bareld Wit, Gero Storeck, and Claus Ropers — IV. Physical Institute, University of Göttingen, Friedrich-Hund-Platz 1, Germany

Metallic nanowires have become a model system for studying correlation effects and light-matter interaction on the atomic scale, providing access to phenomena such as anisotropic conductivity, long-range spin-order or Peierls transitions. Due to their low dimensionality, these systems exhibit a comparatively small number of structural modes, potentially resulting in long dephasing times of optically-excited coherent phonons. Recently, it was shown that single intense light pulses can drive the surface-specific structural phase transition between the insulating (8×2) and the metallic (4×1) phase of In-nanowires on Si(111) in the limit of critically damped atomic motion [1]. Here, we report the coherent control of this structural phase transition enabled by excitation with optical pulse pairs, thereby demonstrating and harnessing pronounced vibrational coherences in the system. A detailed analysis of the phase transition efficiency as a function of the two-pulse delay recorded by ultrafast low-energy electron diffraction (ULEED) [2] proves the critical role of two specific phonon modes for the transition [3], and allows for unique insights to the underlying reaction pathways of this structural phase transition.

[1] T. Frigge et al., Nature 544, 207-211 (2017). [2] S. Vogelgesang

et al., Nat. Physics 14, 184-190 (2018). [3] S. Wippermann et al., PRL 105, 126102 (2010).

O 95.3 Fri 11:00 H14

Excited state mapping and ultrafast population dynamics in In/Si(111) nanowires probed by trARPES — •Chris W. Nicholson[1], Michele Puppin[1], Andreas Lücke[2], Wolf Gero Schmitt[2], Laurenz Rettig[1], Ralph Ernstorfer[1], and Martin Wolf[1] — [1]Fritz Haber Institute, Berlin — [2]University of Paderborn

Ultrafast electronic structure probes allow detailed insights into the microscopic processes underlying photo-induced phase transitions, as recently exemplified by the time- and angle-resolved photoemission spectroscopy (trARPES) study of the model (8x2) to (4x1) structural transition in In/Si(111) nanowires [1].

In this talk, I will address two further aspects of the electronic structure dynamics as probed by our trARPES setup utilizing a 22 eV laser at 500 kHz. The first is the extension of the band-mapping concept to states above the Fermi level, which allows a rigorous benchmarking of band structure calculations in this system. The second is an energy and momentum resolved analysis of the population dynamics during the phase transition. A comparison with a simulated band structure based on a transient electronic temperature finds impressive agreement, supporting the high electronic temperature extracted in the surface layer following excitation. These results are compared to those obtained with femtosecond electron diffraction [2] and imply a non-thermal phonon population of the surface In atoms and suggest a bottleneck for cooling of optical phonons.

[1] Nicholson et al. Science 362, 821 (2018)

[2] Frigge et al. Struct. Dyn. 5, 025101 (2018)

O 95.4 Fri 11:15 H14

1D- plasmons and their H-induced modification on the Si(557)-Au surface — •Zamin Mamiyev[1], Simone Sanna[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [2]Theoretische Physik, Justus-Liebig-Universität Gießen, Gießen

Recently significant progress has been made on metallic atomic wires on the stepped Si surfaces. However, there are still fundamental questions concerning substrate wire interaction, tunability in atomic scale et.c. need to be clarified. Such wires host anisotropic plasmonic excitations which contain significant information about excitated states and also have a potential application in nano-optoelectronics. Here we use plasmon spectroscopy and atomistic DFT calculations to study the H-induced modifications of quasi-1D plasmons in Au atomic wires on the Si(557) surface. Single atomic Au chains per terrace form upon evaporation of 0.19ML Au onto this surface while emerging other structural motifs with an individual chemical potential. Adsorption of atomic H induces a reduction of dispersion and levelling of the dispersion around 0.45 eV for $k_\parallel > 0.08$ Å, indicative of band gap opening in the unoccupied part of the band structure. No extrapolation to E=0 at $k_\parallel = 0$ is possible any more, indicating increased electronic localization and/or influences by disorder. These findings are corroborated by DFT calculations, which predict adsorption of H first on the Si step edge and then on the Si rest atom row. Using the relation between e-h continuum and plasmon dispersion, the modification of band structure and its consequences on plasmonic excitation will be discussed.

O 95.5 Fri 11:30 H14

Temperature induced phase transition of Si(553)-(5x2)-Au in vibrational spectra and its suppression upon step edge hydrogenation — •Eugen Speiser[1], Julian Plaickner[1], Sandhya Chandola[1], Simone Sanna[2], Conor Hogan[3], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V. Schwarzschildstrasse 8, 12489 Berlin, Germany — [2]Institut für Theoretische Physik, Heinrich-Buff-Ring 16, 35392 Gießen — [3]Istituto di Struttura della Materia-CNR (ISM-CNR), via Fosso del Cavaliere 100, 00133 Rome, Italy

Si(553)-(5x2)-Au is known for its combined structural/electronic phase transition, confirmed by calculations and experiments. Its investigation by vibrational spectroscopies is promising due to their unique sensitivity to atomic scale properties. By comparison to DFT calculations, certain modes in vibrational spectra are assigned to the Si step edge and hence can be used for probing its properties. Indeed, we observe a temperature induced change in vibrational modes at the step edge. The properties of this system are governed by the charge distribution between step edge and Au-chain. As shown previously hydrogenation of the step edge opens the possibility to use it for manipulation of charge distribution. We show that hydrogenation of the step edge suppresses the phase transition related change in vibrational modes. A tentative explanation will be given in terms of thermally induced fluctuation in the charge distribution for the non-hydrogenized surface. This fluctuation is inhibited by additional charge, introduced by hydrogen, suppressing the phase transition.

O 95.6 Fri 11:45 H14

Temperature-dependent order-disorder transition in the Si(553)-Au nanowire system — •Bernd Hafke[1], Tobias Witte[1], Christian Brand[1], Simone Sanna[2], Christian Braun[3], Wolf Gero Schmidt[3], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [2]Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [3]Universität Paderborn, Pohlweg 55, 33098 Paderborn

Deposition of 0.5 ML Au on Si(553) at 650 °C results in the formation of Au double-strand metallic chains with a twofold periodicity along the terraces of the vicinal Si surface. The step edge atoms of the Si terraces are characterized by a threefold periodicity, due to the presence of unoccupied dangling bonds [1,2]. The long-range interaction of the twofold and threefold periodicity is investigated by spot-profile analysis in LEED as function of temperature between 60 K and 190 K. The correlation length of Si step edge atoms along and perpendicular to the steps abruptly decreases upon heating above a temperature of $T \approx 100$ K, respectively. These findings are explained within a scenario of an order-disorder transition, where the thermal creation of solitons destroy the long-range ordering. Additionally, time-resolved ultra-fast RHEED experiments show the streak-like intensity, indicative for the twofold periodicity of the Au atoms, to decrease upon intense fs-optical excitation. This indicates transient weakening of the dimerization within the Au double-strand.

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. **1**, 58 (2010).

[2] C. Braun, *et al.* PRB **98**, 121402 (2018).

O 95.7 Fri 12:00 H14

Spin pairing versus spin chains at Si(*hhk*)-Au surfaces — •Christian Braun and Wolf Gero Schmidt — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn

Surfaces involving single spin states are promising candidates for the realization of spin-based computation and storage. Both the Si(553)-Au and Si(557)-Au surface have been discussed to exhibit such unpaired spins for several years [1]. Density-functional theory is used to probe the spin structure of these surfaces. For Si(553)-Au a diamagnetic sp2 + p rehybridized structure, where the dangling bonds are either filled with two spin-paired electrons or are empty, is more favorable and in better agreement with experiment than the generally accepted spin-chain model. In contrast, the spin chains on Si(557)-Au seem rather stable against rehybridization. We discuss the mechanisms for this diverging behavior and predict methods to tailor the existence of single spin states on these surfaces. [2]

[1] S C Erwin, F J Himpsel, Nature Communications 5, **58** (2010)

[2] C Braun, U Gerstmann, W G Schmidt, Physical Review B **98**, 121402 (2018)

O 95.8 Fri 12:15 H14

Phenomenological assignment of surface phonons at Si(hhk) modified by Au submonolayers — •Julian Plaickner[1], Eugen Speiser[1], Sandhya Chandola[1], Nobert Esser[1], Benedikt Halbig[2], and Jean Geurts[2] — [1]Leibniz-Institut für Analytische Wissenschaften-ISAS- e.V. Schwarzschildstrasse 8, 12489 Berlin, Germany — [2]Universität Würzburg, Physikalisches Institut, Experimentelle Physik 3 Am Hubland, 97074 Würzburg, Germany

Raman spectroscopy is an extremely sensitive tool for analyzing vibration modes of ordered (sub)monolayers of metal adatoms on semiconductor surfaces, which are typical systems for electron correlation effects. We report on the in situ UHV Raman analysis of self-organized Au submonolayers on nominal Si(111) surfaces, as well as on vicinal Si(553), Si(775), and Si(557). For the two-dimensional Au-(sqrt(3)xsqrt(3)) and the one-dimensional Au-(5x2) reconstructions, several specific Raman peaks in the spectral range below 200 cm-1 are assigned to Au-dominated vibrational modes, while Si-step-edge vibrational modes around 400 cm-1 are fingerprints of the substrate orientation.

O 95.9 Fri 12:30 H14

Tb induced surface structures on Si(110) — •Stephan Appelfeller and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Metallic rare earth silicide nanostructures are known to form by deposition of rare earth elements on clean Si substrates and annealing. The growth of nanowires is observed on Si(001) substrates due to anisotropic strain and on Si(*hhk*) substrates due to steps disrupting the two-dimensional film growth found on Si(111) substrates. Such rare earth silicide nanowires are not only interesting for studying the unique one-dimensional physics, but are also promising for future applications since they consist of the metallic bulk silicides, possibly allowing their passivation by capping without strong changes of their properties.

Here, the growth of Tb induced surface structures on the Si(110) surface is studied. Using scanning tunneling microscopy, single domain growth of Tb silicide structures with very high aspect ratios, i.e. of Tb silicide nanowires, is observed even on planar substrates due to its structural anisotropy. Furthermore, scanning tunneling spectroscopy clearly shows that these nanowires have a finite density of states at the Fermi level. In contrast, the wetting layer, which accompanies the nanowires formation, is characterized by a small band gap. This wetting layer is also studied using low energy electron diffraction revealing the formation of two domains.

This work was supported by the DFG, FOR 1700, project E2.

O 95.10 Fri 12:45 H14

Charge density wave melting in one-dimensional wires with femtosecond sub-gap excitation — •Mariana Chávez-Cervantes, Gabriel E. Topp, Sven Aeschlimann, Răzvan Krause, Shunsuke A. Sato, Michael A. Sentef, and Isabella Gierz — Max Planck Institute for the Structure and Dynamics of Matter

Charge density waves (CDWs) are symmetry-broken ground states that commonly occur in low-dimensional metals due to strong electron-electron and /or electron-phonon coupling. The non-equilibrium carrier distribution established via photodoping with femtosecond laser pulses readily quenches these ground states and induces an ultrafast insulator-to-metal phase transition. To date, CDW melting has been mainly investigated in the single-photon and tunneling regimes, while the intermediate multi-photon regime has received little attention. Here we excite one-dimensional indium wires with a CDW gap of 300 meV with mid-infrared pulses at 190 meV with MV/cm field strength and probe the transient electronic structure with time- and angle-resolved photoemission spectroscopy (tr-ARPES). We find that the CDW gap is filled on a timescale short compared to our temporal resolution of 300 fs and that the phase transition is completed within 1 ps. Supported by a minimal theoretical model we attribute our findings to multi-photon absorption across the CDW gap.

O 96: Focus Session: Surface Transport at the Atomic Scale

The ability to probe electronic transport on nano- and even atomic scaled structures opened a new field. Besides break junction techniques for realizing 2-terminal transport setups, recently, also multiprobe technique based on scanning tunneling microcopy (STM) allowed to go beyond and demonstrated its capability to reveal fundamental charge transport properties. This Focus Session will give an brief overview over the progress made on various topics with surface transport, ranging from functionalized semiconductor surfaces, 2D materials, topological insulators, helical molecules down to atomic wires.

Organizers: Christoph Tegenkamp (TU Chemnitz) and Bert Voigtländer (FZ Jülich).

Time: Friday 10:30–13:00 Location: H15

Invited Talk O 96.1 Fri 10:30 H15

Electrical transport in semiconductor nanocrystal assemblies and nanocrystal heterostructures — •Bruno Grandidier — IEMN-CNRS, Dept. ISEN Physics, 41 bd Vauban, 59000 Lille, France

Structures consisting of semiconductor nanocrystals are solution-processable materials that are prized for the low-cost and scalability of their fabrication method and their compatibility with flexible, thin-film electronics. Their transport properties are governed by the interfaces between the nanocrystals themselves or the nanocrystals and the supporting semiconductor substrates. Here we will investigate both types of interfaces. We will show how the direct attachment of nanocrystals via chemical bonds between atoms instead of linkage via carbon-based molecules significantly improves the conductivity of two-dimensional nanocrystal arrays. In these systems, charges are coherently delocalized along nanometer-scale segments of nanocrystals ensuring a high THz mobility, while the DC mobility is limited by the absence of long-range order in the arrays. As to solution-based nanocrystal-semiconductor heterostructures, we will show how an initial wet chemical passivation step before the epitaxial growth of the nanocrystals on semiconductor substrates is key not only to produce an atomically sharp crystalline interface, but also to form trap-free interfaces with quality comparable to that grown by molecular beam epitaxy.

O 96.2 Fri 11:00 H15

Space-charge layer effects studies by surface transport — •Frederik Edler[1,2], Ilio Miccoli[2], Herbert Pfnür[2], and Christoph Tegenkamp[1,2] — [1]Institut für Festkörperphysik, Technische Universität Chemnitz, 09126 Chemnitz — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover

Electronic properties of low dimensional structures on surfaces can be comprehensively explored by surface transport experiments, e.g., giving a direct access to instability-driven metal insulator transitions. However, the surface sensitivity of this technique to atomic structures comes along with the control of bulk related electron paths and internal interfaces. We analyzed the role of Schottky-barriers and space charge layers for Si-surfaces. By means of a metal submonolayer coverage deposited on vicinal Si(111), we reliably accessed subsurface transport channels via angle- and temperature-dependent in-situ transport measurements. In particular, we show that high temperature treatments performed under even ultra high vacuum conditions lead to the formation of surface-near bulk defects, e.g. SiC interstitials. These defects act as p-type dopants and easily overcompensate pristine low dopant concentrations in Si. This effect is of high significance in low-doped Si samples.

O 96.3 Fri 11:15 H15

In-situ four-tip STM investigation of the transition from 2D to 3D charge transport in SrTiO3 — •Arthur Leis[1,2], Christian Rodenbücher[1,2], Krzysztof Szot[1,2], Vasily Cherepanov[1,2], F. Stefan Tautz[1,2], and Bert Voigtländer[1,2] — [1]Peter Grünberg Institut (PGI-3, PGI-7), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, Germany

The electrical properties of SrTiO3(100) single crystals were investigated in-situ at different stages of thermal reduction by means of a 4-tip STM. Using the tips of the STM as electrical probes, distance-dependent four-point measurements were performed at the surface of the crystal at room temperature after reduction by thermal treatment. For annealing temperatures $T < 700^\circ$C, charge transport is confined to a surface region < 3mm below the surface. For reduction at $T > 900^\circ$C a transition from a conducting 2D sheet with insulating bulk to a system with dominant 3D bulk conductivity is found. At an intermediate reduction temperature of $T = 800^\circ$C, a regime with mixed 2D/3D contributions is observed in the distance-dependent resistance measurements. Describing the depth dependent conductivity with an analytical N-layer model, this regime of mixed 2D/3D conductivity is evaluated quantitatively under the assumption of an exponentially decaying conductivity profile, correlated with the previously observed depth dependent dislocation density in the sample. A non-monotonous temperature dependence of the 3D conductivity in the respective conducting layer is found and the underlying mechanism is discussed.

O 96.4 Fri 11:30 H15

Length dependent electrical transport trough single polyalanine molecules — •Diana Slawig[1], Nguyen Thi Ngoc Ha[2], Herbert Pfnür[1], and Christoph Tegenkamp[1,2] — [1]Leibniz Universität Hannover — [2]TU Chemnitz

A new promising and effective approach for spintronics has emerged using spin selectivity in electron transport through chiral molecules, named Chiral Induced Spin Selectivity (CISS)[1]. Recently, by utilizing this effect a proof of concept for a new type of chiral-based Si-compatible universal magnetic memory device was demonstrated[2]. Nevertheless, the electrical transport through helical peptides itself is not completely understood yet. Our study focuses on transport through single polyalanine (PA) molecules by means of mechanically controlled break junctions.

Transport measurements for PA molecules consisting of 16- and 36 monomers revealed two characteristic conductions values accompanied by satellite peaks. The length dependence of the conductance revealed an exponential decay pointing towards tunneling. Moreover, this lengths distribution see in transport correlates nicely with STM investigations showing also PA molecules of various lengths. The conductance through these molecules is comparably high and indicates that superexchange tunnelling may play a role.

[1]R. Naaman et.al., ,J. Phys. Chem. Lett., 3 (2012)
[2]O. Ben Dor et.al.Nat. Commun. 4:2256 (2013)

Invited Talk O 96.5 Fri 11:45 H15

Multiprobe STM measurements of electron transport at the atomic level — •Marek Kolmer, Wonhee Ko, and An-Ping Li — Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

Techniques based on multiprobe scanning tunneling microscopy (MP-STM) allow determination of electronic and spin transport in variety of systems supported on surfaces of solid materials. These MP-STM methods are currently considered as universal tools for in-situ characterization of mesoscopic transport phenomena in scales down to hundreds of nanometers. Alternatively, application of scanning tunneling potentiometry visualizes potential change during such mesoscopic charge current transport with a nominal nm resolution.

Here, we would like to discuss our efforts towards changing of this mesoscopic experimental paradigm by downscaling MP-STM experiments to the atomic level. In this case charge or spin current supplying probes are positioned in atomically defined locations with respect to the characterized nanosystem. Our experiments rely on fully STM-based tip positioning protocol with probe-to-probe separation distances reaching tens of nm. This is combined with about 5 pm vertical sensitivity in probe-to-system contact definitions. Those two factors enable realization of multiprobe scanning tunneling spectroscopy experiments, where transport properties could be characterized by macroscopic probes kept in well-defined tunneling conditions.

This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

O 96.6 Fri 12:15 H15

Parallel conduction channels in topological insulator thin films: Role of the interface layer and the band bending in the film — •Sven Just[2,3], Felix Lüpke[4], Stefan Korte[1], Vasily Cherepanov[1], Frank Stefan Tautz[1], and Bert Voigtländer[1] — [1]Peter Grünberg Institute (PGI-3) and JARA-FIT, Forschungszentrum Jülich, Germany — [2]II. Physikalisches Institut B, RWTH Aachen, Germany — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Germany — [4]Departement of Physics, Carnegie Mellon University, Pittsburgh, PA 15213, USA

Topological insulator (TI) thin films can exhibit multiple parallel channels for current transport: beside the topological surface states (TSS), e.g. the interior of the TI film, the interface layer and the substrate. A crucial task is to minimize the influence of the parasitic channels for taking advantage of the TSS properties. We present a method for determining the conductivity of the interface between substrate and TI film by distance-dependent surface-sensitive four-probe measurements with a multi-tip STM. Moreover, as the conductivity of the interior of the TI thin film (bulk) is difficult to access by measurements, we propose here an approach for calculating the near-surface band bending and the mobile charge carrier density inside the TI thin film based on data from surface-sensitive measurements, e.g. (gate-dependent) four-point resistance measurements and ARPES. It turns out that in the thin-film limit the band-bending is largely independent on the dopant concentration of the film, which allows to estimate the total mobile charge carrier density and the conductivity of the TI thin film.

O 96.7 Fri 12:30 H15

In-situ disentangling surface state transport channels of a topological insulator thin film by gating — •Bert Voigtländer, Felix Lüpke, Sven Just, Vasily Cherepanov, and F. Stefan Tautz — Peter Grünberg Institut (PGI-3) and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany

In the thin film limit, the surface state of a three-dimensional topological insulator gives rise to two parallel conduction channels at the top and bottom surface of the film, which are difficult to disentangle in transport experiments. Here, we present gate-dependent multi-tip scanning tunneling microscope transport measurements combined with photoemission experiments all performed in-situ on pristine BiSbTe3 thin films. To analyze the data, we develop a generic transport model including quantum capacitance effects. This approach allows us to quantify the gate-dependent conductivities, charge carrier concentrations, and mobilities for all relevant transport channels of three-dimensional topological insulator thin films (i.e., the two topological surface state channels, as well as the interior of the film). For the present sample, we find that the conductivity in the bottom surface state channel is minimized below a gate voltage of V = *34 V and the top surface state channel dominates the transport through the film.

O 96.8 Fri 12:45 H15

Exploring the unjamming of electrons with a multi-probe STM — •Yaroslav Gerasimenko[1,2], Michele Diego[2], Jan Ravnik[2], and Dragan Mihailovic[1,2] — [1]CENN Nanocenter, Jamova 39, 1000, Ljubljana, Slovenia — [2]Department of Complex Matter, Jozef Stefan Institute, Jamova 39, 1000, Ljubljana, Slovenia

The combination of a multi-probe STM and an in situ ultrafast excitation allows us to explore novel states of matter that can emerge from many-body interactions under highly non-equilibrium conditions. Here we show that a single femtosecond-scale optical pulse, applied to the prototypical transition metal dichalcogenide 1T-TaS$_2$, can convert a perfect hexagonal charge order into an exotic metastable amorphous jammed state of strongly correlated electrons [1].

Tunnelling spectra and four-probe surface transport measurements reveal a remarkable duality of localized and itinerant charges in this state. While the latter are predominantly responsible for hopping conductivity, the potential landscape is provided by the former ones. As the jammed state starts to relax at higher temperatures, consecutive STM images reveal the onset of the diffusion of the previously localised charges. By matching it with the multi-probe resistivity measurements, we identify a highly unusual dynamical regime in the surface transport.

[1] Ya. A. Gerasimenko, I. Vaskivskyi, J. Ravnik, J. Vodeb, V. Kabanov, D. Mihailovic, Quantum jamming transition to a correlated electron glass in 1T-TaS$_2$, arXiv:1803.00255 (2018)

O 97: Ultrafast Electron Dynamics at Surfaces and Interfaces III

Time: Friday 10:30–13:00 Location: H16

O 97.1 Fri 10:30 H16

The transient modification of a ZnO surface upon photoexcitation — •Lukas Gierster, Sesha Vempati, and Julia Stähler — Fritz-Haber-Institut Berlin, Dpt. Phys. Chem.

ZnO is intensely explored due to its great potential especially in the field of optoelectronics and (photo-) chemistry. However, it is still under debate how the properties of ZnO vary with photoexcitation [1]. Here, we use time- and angle resolved photoelectron spectroscopy to investigate the transient electronic properties of the ZnO (10-10) surface under resonant photoexcitation of the band gap. At low excitation densities, a small additional signal below the Fermi level is observed, consistent with the previously observed surface exciton formation [2]. Above the Mott density, within about 60 fs an intense spectral feature builds up which exhibits the characteristics of a thermalized electron gas. Likely, this new state results from bending the conduction band below the Fermi level by band gap renormalization: The ZnO surface becomes transiently metallic for hundreds of picoseconds. For all excitation densities a fraction of the pump-induced electronic population survives the inverse repetition rate of the laser (5 μs). The photostationary population must be stabilized by a positive localized charge. Potential candidates are defects and photogenerated hole polarons, as recently observed for ZnO (10-10) [1]. [1] H. Sezen et al, Nat. Comm. 6, 6901 (2015) [2] J.-C. Deinert et al., PRL 113, 057602 (2014)

O 97.2 Fri 10:45 H16

Time Resolved Photoemission Study of the Charge Transfer Dynamics in Anatase TiO2(101) for CO Photooxidation to CO2 — •Michael Wagstaffe[1], Heshmat Noei[1], Simon Chung[1], Lukas Wenthaus[2,3], Guilherme Semione[1], Steffen Palutke[2,3], Giuseppe Mercurio[2,3], Siarhei Dziarzhytski[1], Harald Redlin[1], Nicolai Klemke[2], Yudong Yang[2], Anne-Laure Calendron[2], Franz Kärtner[2], Wilfried Wurth[1,2,3], and Andreas Stierle[1,3] — [1]Deutsches Elektronen-Synchrotron, Notkestr. 85, 22607 Hamburg, Germany — [2]Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Department Physik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

Until recently, severe limitations have been placed on understanding the behavior of the photogenerated charge carriers in the photooxidation of CO to CO2 on TiO2 surfaces due to the ultrafast nature of the reaction. With their unprecedented temporal resolution, FELs allowed new insight to be obtained that has hitherto been unattainable. 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 on anatase 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. For the first time, the photooxidation of CO to CO2 has been observed at two distinct time points of 2.1 ps and 7.3 ps, which we attribute to the charge carriers interacting with different adsorption modes of O2 on the surface.

O 97.3 Fri 11:00 H16

Probing long-range structural dynamics of surfaces by umklapp process assisted time-resolved low-energy photoelectron spectroscopy — •Stephan Jauernik, Petra Hein, Max Gurgel, Julian Falke, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

Laser-based angle-resolved photoelectron spectroscopy is performed on tin-phthalocyanine (SnPc) adsorbed on silver Ag(111). Upon adsorption of SnPc, strongly dispersing bands are observed which are identified as secondary Mahan cones formed by surface umklapp processes acting on photoelectrons from the silver substrate as they transit through the ordered adsorbate layer. We show that the photoemission data carry quantitative structural information on the adsorbate layer similar to what can be obtained from a conventional low-energy electron diffraction (LEED) study. More specifically, we compare photoemission data and LEED data probing an incommensurate-to-commensurate structural phase transition of the adsorbate layer. Based on our results we propose that Mahan-cone spectroscopy operated in a pump-probe configuration can be used in the future to probe structural dynamics at surfaces with a temporal resolution in the sub-100-fs regime.

[1] S. Jauernik, P. Hein et al., Phys. Rev. B 97, 125413 (2018)
[2] G.D. Mahan, Phys. Rev. B 2, 4334 (1970)

O 97.4 Fri 11:15 H16

Exciton dynamics and energy transfer at PTCDA/noble-metal interfaces — •Klaus Stallberg and Ulrich Höfer — Fachbereich Physik, Philipps-Universität, D-35032 Marburg

Combining time-resolved photoluminescence (TRPL) and two-photon photoemission (2PPE) we investigate thin layered films of PTCDA on the (111) surfaces of silver and gold. Our combined experimental approach enables us to study the exciton dynamics from optical excitation in the organic layers to annihilation at the organic/metal interface. More specifically, we identify three different excitonic states – a monomer-related Frenkel exciton, a charge-transfer (CT) exciton, and an excimer – based on their spectral signatures and their radiative lifetimes in TRPL. 2PPE spectra of the same samples exhibit distinct low-energy features which we attribute to hot conduction electrons at the metal surfaces. The exciton dynamics, as probed with TRPL, strongly depends on the PTCDA film thickness which is varied from several nanometers down to a single monolayer. The decrease of the CT exciton radiative lifetime with decreasing film thickness is explained in terms of exciton diffusion along the stacking direction of the PTCDA molecules. Interestingly, exactly the same dependence on the PTCDA film thickness is observed for the hot-electron dynamics, as probed with 2PPE. This strongly points to the CT excitons as source of hot electrons after diffusion to the organic/metal interface. This energy transfer is found much more efficient on Ag(111) than on Au(111) indicating involvement of the metal–organic interface state of PTCDA/Ag(111) which is absent at the PTCDA/Au(111) interface.

O 97.5 Fri 11:30 H16

Ultrafast charge carrier dynamics at the interface F4TCNQ:H-Si(111) from real-time TDDFT — •Matheus Jacobs, Jannis Krumland, Ana M. Valencia, and Caterina Cocchi — Institut fur Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

The electronic structure of inorganic surfaces can be effectively modified by the adsorption of molecular acceptors acting as dopants. As a result, their interaction with light can give rise to charge-transfer excitations at the interface, making the systems potentially appealing for optoelectronic applications. To this end, gaining insight and control on the dynamics of the photo-excited charge-carrier population is an essential task. Here, we consider the interface formed by the strong electron acceptor F4TCNQ adsorbed on the hydrogenated Si(111) surface, which was recently characterized both theoretically and experimentally [1]. The linear absorption spectrum of this system exhibits two maxima in the visible region corresponding to transitions between electronic states hybridized across the interface. In the framework of real-time time dependent density functional theory, as implemented in the octopus code [2], we investigate the charge-carries dynamics induced by a laser pulse in resonance with each excitation and analyze the time evolution of the photoexcited electronic population. Our results offer insight into the earliest stage formation of optical excitations at hybrid interfaces.

[1] H. Wang, et al. arXiv:1811.00037 (2018).
[2] A. Castro, et al. Phys. Stat. Sol. B 243, 2465 (2006)

O 97.6 Fri 11:45 H16

Relaxation of electronically confined states from Master Equation with first-principles-derived rates — •Peter Kratzer, Maedeh Zahedifar, and Sebastian Schreiber — Fakultät für Physik, Universität Duisburg-Essen

Atomically thin films of Pb on Si(111) provide an experimentally tunable system comprising both dispersive bands with metallic character and confined, thickness-dependent quantum well states. The lifetime of excited electrons in Pb films is limited by both electron-electron (e-e) and electron-phonon (e-ph) scattering. We employ the description by a Master equation for the electronic occupation numbers to analyse the relative importance of both scattering mechanisms. The electronic and phononic band structures, as well as the matrix elements for electron-phonon coupling within deformation potential theory were obtained from density functional calculations. The contribution of impact ionization processes to the lifetime is estimated from the imaginary part of the electronic self-energy calculated in the GW approximation. By numerically solving the rate equations for the occupations of the Pb-derived electronic states coupled to phononic heat baths, we can follow the distribution of the electronic excitation energy to the various modes of Pb lattice vibrations. While e-e scattering is the dominant relaxation mechanism, we demonstrate that the e-ph scattering is highly mode-selective, with a large contribution from surface phonons. The time scales extracted from the simulations are compared to experimental data from time-resolved pump-probe experiments.

Funding: DFG, SFB1242

O 97.7 Fri 12:00 H16

Resonant charge transfer and energy dissipation during scattering of H$^+$/Al(111) studied with TDDFT and adiabatic GGA — •Lukas Deuchler, Christopher Makait, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, CAU Kiel, Germany

Ab initio molecular dynamic simulations employing time-dependent density functional theory to describe the electron dynamics combined with Ehrenfest dynamics for the nuclei [1] within the limitation due to the approximate XC potential facilitate the investigation of resonant charge transfer during ion neutralization and electron-hole pair excitation at surfaces [2]. We have studied the scattering of hyperthermal H$^+$ and H/Al(111) (for which experimental [3] and theoretical [4,5] results are available for comparison). Simulations have been performed with the code octopus [1] by A. Rubio et al. Charge and energy transfer and the excitation spectra have been compared for H$^+$ and H impinging on the Al substrate. Tight-binding simulations [6] with input derived from TDDFT are capable of reproducing the charge transfer dynamics. In-detail analysis of the simulation results allows to pinpoint remaining open questions.

[1] Andrade et al., Phys Chem Chem Phys **17**, 31371 (2015),
[2] Zhao et al., Phys Condens Matter **27**, 025401 (2015),
[3] Winter, Phys Condens Matter **8**, 10149 (1996),
[4] Merino et al., Phys Rev B **54**, 15 (1996),
[5] Lindenblatt et al., Nucl Instrum Meth Phys B **246**, 333 (2006),
[6] Brako and Newns, Vacuum **32**, 1 (1982).

O 97.8 Fri 12:15 H16

Microscopic energy flow dynamics in Fe/MgO — •Nico Rothenbach[1], Markus E. Gruner[1], Katharina Ollefs[1], Ping Zhou[1], Carolin Schmitz-Antoniak[2], Niko Pontius[3], Rolf Mitzner[3], Christian Schüssler-Langeheine[3], Rossitza Pentcheva[1], Klaus Sokolowski-Tinten[1], Renkai Li[4], Mianzhen Mo[4], Suji Park[4], Xiaozhen Shen[4], Stephen Weathersby[4], Jie Yang[4], Xijie Wang[4], Heiko Wende[1], Uwe Bovensiepen[1], and Andrea Eschenlohr[1] — [1]University Duisburg-Essen and CENIDE — [2]FZ Jülich — [3]Helmholtz-Zentrum Berlin — [4]SLAC

A localized optical excitation of a metal/insulator heterostructure, like a Fe/MgO multilayer, by a femtosecond (fs) laser pulse induces ultrafast dynamics like charge and spin transfer processes as well as coupling to low energy excitations mediated by e.g. electron-electron and electron-phonon scattering. We measure fs time- and element-resolved soft x-ray spectroscopy to separate and identify the electronic and lattice excitations. The latter is also analyzed by complementary ultrafast electron diffraction experiments. The response at the Fe L$_3$-edge is maximal at 200 fs and represents local electronic excitations, coupling to phonons in Fe, and their relaxation to the insulator. The dynamics at the O K-edge reaches a maximal change after 400 fs, explained by lattice excitations of MgO due to energy transfer from Fe. Probing the O pre-edge gives rise to the interface states dynamics and deepens our understanding further. DFT calculations of layer-resolved vibrational and electronic DOS consolidate our interpretation. We acknowledge financial support by the DFG through the SFB1242.

O 97.9 Fri 12:30 H16

Dynamics of optical excitations in a Fe/MgO(001) heterostructure from time-dependent density functional theory — •Markus Ernst Gruner, Elaheh Shomali, and Rossitza Pentcheva — Faculty of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen, Germany

In the framework of real-time time-dependent density functional theory (RT-TDDFT) we unravel the layer-resolved dynamics of the electronic structure of a (Fe)$_1$/(MgO)$_3$(001) multilayer system after an optical excitation with a frequency below the band gap of bulk MgO. Substantial transient changes to the electronic structure, which persist after the duration of the pulse, are observed in particular for in-plane polarized electric fields, corresponding to a laser pulse arriving perpendicular to the interface. While the strongest charge redistribution takes place in the Fe layer, a time-dependent change in the occupation numbers is visible in all layers, mediated by the presence of interface states. The time evolution of the layer-resolved occupation numbers indicates a strong orbital dependence with the depletion from in-plane orbitals (e.g. $d_{x^2-y^2}$ of Fe) and accumulation in out-of-plane orbitals (d_{z^2} of Fe and p_z of apical oxygen). We also see a small net charge transfer away from oxygen towards the Mg sites even for MgO layers, which are not directly in contact with the metallic Fe.

Financial support from the DFG within SFB 1242 (project C02) is gratefully acknowledged.

O 97.10 Fri 12:45 H16

Local and Non-Local Relaxation Dynamics of Hot Electrons in Au/Fe/MgO(001) — •Yasin Beyazit[1], Jan Beckord[1], John Thomas[1], Ping Zhou[1], Detlef Diesing[2], Manuel Ligges[1], and Uwe Bovensiepen[1] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Faculty of Chemistry, University of Duisburg-Essen, 45141 Essen, Germany

Photo-excited, hot electrons in multilayer thin films exhibit local and non-local dynamics which lead to relaxation and transport effects. The investigation of their interplay is so far mainly based on all-optical measurements. We present a novel tool for energy-resolved analysis of local and non-local relaxation dynamics in condensed matter. By using a back-pump/front-probe experimental configuration in femtosecond time-resolved, two-photon photoemission (tr-2PPE), we aim at separating these relaxation processes. The tr-2PPE intensity provides the relaxation time τ and the delay of the maximum intensity t^*, and, thus, independent observables which we discuss in terms of inelastic relaxation and ballistic transport. We show first results for Au/Fe/MgO(001) and (i) τ as a function of energy $E - E_F$ as well as Au thickness d_{Au} and (ii) t^* regarding energy-resolved transport velocities of hot electrons. The proportionality between t^* and Au thickness points strongly towards ballistic transport. Our obtained velocities are in a good agreement with the literature values. This study was funded by the DFG through SFB1242.

O 98: Organic Molecules on Inorganic Substrates VII

Time: Friday 10:30–12:15 Location: H17

O 98.1 Fri 10:30 H17

An Electro Spray Ion Beam Deposition Device Employing Novel Ion Guide Concepts — •Andreas Walz, Peter Knecht, Karolina Stoiber, Hartmut Schlichting, and Johannes Barth — Physics Department E20, Technical University of Munich, Germany

The world of nanostructures requires precise control and growth of atomically clean films of clusters or molecules on well-defined surfaces. Most state of the art techniques like organic molecular beam epitaxy are limited to small and sublimable clusters or molecules. Electro Spray Controlled Ion Beam Deposition (ES-CIBD) gives access to reactive, larger and thermolabile species including many biomolecules. However, near ambient conditions for the generation of ions via electro spray ionization conflict with the ultra-high vacuum routinely required for the deposition via soft-landing and subsequent investigations. The challenge is to overcome pressure differences of 13 orders of magnitude while preserving high ion flux for appropriate preparation times as well as precise control of the deposited species.

Here we introduce advanced radio frequency ion optics combining highly efficient ion transmission with extremely low neutral gas leakage. We present a modified stacked ring ion guide combined with a novel high order multipole - the Small Wire Ion Guide (SWIG) - and a blade ion guide. The mass of the deposited species is determined by a digital quadrupole mass spectrometer with adjustable frequency and nearly unlimited mass range. Simulations using the software package SIMION have assisted the design. The deposited layers have been investigated with scanning tunneling microscopy.

O 98.2 Fri 10:45 H17

Physical decoupling of tetrapyrrolic metal-organic complexes on metal surfaces via self-assembled monolayers — Peter S. Deimel, Peter Feulner, Johannes V. Barth, and •Francesco Allegretti — Physik Department E20, Technische Universität München, Deutschland

Tuning the electronic properties of metal-organic complexes such as metalloporphyrins (MPs) and metallophthalocyanines (MPcs) holds promise for their targeted application in, e.g., photocatalysis and molecular sensors. In such cases, the complexes will be “immobilized” on solid supports, and for such reason numerous studies have focused on their adsorption on model metal surfaces in vacuo. As MPs and MPcs typically adsorb with their tetrapyrrole macrocycle almost parallel to the metal surface, the interaction between the latter and the central metal ion can decisively alter the chemical and functional properties of the adsorbed complex and even quench its reactivity. Herein we explore a simple strategy to decouple, both spatially and electronically, two prototypical Fe-phthalocyanine and Ru-porphyrin monolayers from a Ag(111) surface, by preventing direct physical contact with the Ag support via insertion of a self-assembled monolayer (SAM) of fluorothiophenol. By combining photoelectron spectroscopy, temperature programmed desorption and low-energy electron diffraction, we show that at low temperatures the thiolate SAM indeed acts as molecular spacer layer. However, already below 300 K, the decoupling breaks down, resulting in an inverted layer stacking followed by complete removal of the SAM molecules at elevated temperatures.

O 98.3 Fri 11:00 H17

Tuning TCNQ adsorption on Ag(100): A joint DFT and experiment study of the role of alkali coadsorption — •Billal Sohail[1], Luke Rochford[2], Phil Blowey[1], Phil Woodruff[3], Giovanni Costantini[1], and Reinhard J. Maurer[1] — [1]Department of Chemistry, University of Warwick, UK — [2]School of Chemistry, University of Birmingham, UK — [3]Department of Physics, University of Warwick, UK

TCNQ (7,7,8,8-tetracyanoquinodimethane) is a well established electron acceptor with an innate ability to form conductive organic salts. Interest in the multidisciplinary field of molecular electronics has piqued due to the variety of applications such as, organic photovoltaics (OPVs), organic field effect transistors (OFETs). Adsorbed on coinage metal surfaces, computational efforts find TCNQ adopts a specific geometry with the peripheral cyano groups bent toward the metal surface, which is lifted upon coadsorption with potassium. We present joint computational and experimental efforts to examine the intricate coupling of structure and electronic structure for TCNQ coadsorbed with potassium atoms on Ag(100) surfaces. By combining many-body-dispersion-inclusive Density-Functional Theory [1] and x-ray standing wave (XSW) and STM measurements, we arrive at a comprehensive picture of structure and stability as determined by the balance of molecule-metal and molecule-molecule charge-transfer and dispersion interactions. [1] Maurer et al., J. Chem. Phys., **143**, 102808 (2015);

O 98.4 Fri 11:15 H17

Understanding Charge Transfer of TCNE on Cu(111) using Structure Search — •Alexander T. Egger[1], Lukas Hörmann[1], Andreas Jeindl[1], Milica Todorović[2], Patrick Rinke[2], and Oliver T. Hofmann[1] — [1]Institute of Solid State Physics, TU Graz, Austria — [2]Department of Applied Physics, Aalto University, Finland

TCNE (tetracyanoethene) is known as a strong electron acceptor that forms charge-transfer complexes upon adsorption on metals. On Cu(111), it has been claimed [1] that this charge transfer includes the second layer, whereby molecules of this second layer are singly charged.

To understand these charge-transfer complexes, knowing the atomic structure of the adlayers is mandatory. However, the number of possible geometries is immense and an accurate describtion of charge transfer requires dispersion-corrected density functional theory (DFT), which – due to its computational costs – inhibits a brute-force search. Using two complimentary machine-learning-based approaches [2,3] allows us to predict the adsorption energies of an exhaustive set of coarse-grained candidate structures at reasonable computational cost while preserving the numerical accuracy of the electronic structure calculations.

Our studies reveal that for TCNE on Cu(111) charge transfer to the second layer is in fact negligible. Instead, a phase transition occurs in the first layer: At high coverage adsorbate molecules flip from face-on to edge-on orientation explaining the observed singly-charged species.

[1] Erley et al., J. Phys. Chem., 91.11
[2] Hörmann et al., arXiv:1811.11702
[3] Todorović et al., arXiv:1708.09274

O 98.5 Fri 11:30 H17

Surface polymorph formation explained: Acenequinones on Ag (111) — •Andreas Jeindl, Lukas Hörmann, Alexander T. Egger, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Understanding (and modifying) the formation of surface polymorphs is still not straightforward, as it is hardly known why specific structures form. Experimental studies are hindered by the huge thermodynamic search space and kinetic trapping. Computational studies, on the other hand, are hampered by the so-called ’configurational explosion’.

In this contribution, we computationally investigate the formation of surface polymorphs for a homologous series of acenequinones on Ag (111). We perform a comprehensive structure search utilizing the SAMPLE[1,2] approach, which combines a physically-motivated coarse graining of the potential energy surface with machine learning to overcome the configurational explosion.

Contrary to most machine learning methods, which rely on mere statistical correlation, our approach gives valuable physical insight into the systems of interest. We investigate the interactions of low-energy polymorphs, distinguishing between inter-molecular and molecule-surface interactions. For further insight, we map the interactions onto different parts of the molecules, which allows us to identify the main contributors of polymorph formation. This could serve as a first step towards establishing rules for a systematic design of surface layers.

[1] Hörmann et al., arXiv:1811.11702
[2] Scherbela et al., Phys. Rev. Materials 2, 043803

O 98.6 Fri 11:45 H17

Hybrid nanoassemblies of ordered nanoparticles and perylene — •Natalia Alyabyeva, Aimeric Ouvrard, and Bernard Bourguignon — Institut des Sciences Moléculaires d’Orsay (ISMO), CNRS, Université Paris-Saclay, 91405 Orsay, France

We demonstrate ordering of hybrid assemblies of Pd nanoparticles (NPs) and perylene on Al2O3/Ni3Al(111). Multi-scale surface science techniques provide a complete description of this system. Scanning tunnelling microscopy (STM) probe topography, adsorption sites and local density of states, while differential reflectance spectroscopy

(DRS) and sum frequency generation (SFG) give access to molecular orientation, coverage and thickness. Different adsorption phases of perylene on alumina depending on coverage and the presence of NPs have been observed. Perylene organizations on bare alumina are in registry with the substrate, evidencing the balanced interplays of molecule-substrate and intermolecular interactions. Molecules are flat-laying at low coverage and up-standing when the layer densifies as well as in the multilayer regime. Ordered hybrid assemblies can be formed where perylene is flat-laying in between NPs smaller than 1 nm. For larger coverage and NP size, perylene is up-standing and also adsorbing on NPs. Disorder progressively appears, showing that NPs hinders long-range intermolecular interactions. Adsorption on NPs leads to a larger SFG signal and a different electronic structure as observed by DRS and STM. Ordered NPs and molecules offer a way to tune electronic, chemical, and optical properties to build optimal architectures for future nanoelectronic devices.

O 98.7 Fri 12:00 H17

Injection-tuning at metal-semiconductor interfaces to boost organic electronics — •Florian von Wrochem[1] and Maria Anita Rampi[2] — [1]Materials Science Laboratory, Sony Europe, Stuttgart (Germany) — [2]Universita di Ferrara, Ferrara (Italy)

The driving force in molecular electronics within the past decades has been to shift organic-based thin-film devices from basic research to the application level. In this talk, a few strategies toward the realization of organic electronic devices on the basis of ultrathin functional organic layers are outlined, specifically by leveraging on the self-assembly process at interfaces. In the first place, we show how large area molecular junctions of outstanding robustness can be realized using densely packed molecular metal-terpyridine complex oligomers, which might enable a versatile platform for functional optoelectronic layers. In the second part, a new class of self-assembled monolayers exhibiting a pronounced intrinsic dipole moment is presented, by which the injection properties in organic semiconductors can be tuned in view of in solar cell and organic memory applications.

O 99: Focus Session: Spins on Surfaces III (joint session O/MA)

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

Invited Talk O 99.1 Fri 10:30 H24

Quantum simulation through atomic assembly — •Sander Otte — Delft University of Technology, Delft, The Netherlands

The magnetic and electronic properties of materials often find their origin in basic atomic- scale interactions. Yet, due to the large number of atoms involved, many phenomena can be very difficult to predict: we call these 'emergent'. The ability to build structures atom-by-atom by means of scanning tunneling microscopy (STM) provides an excellent platform to explore emergence as a function of system size. By properly tuning the anisotropy and coupling of magnetic atoms on a thin insulator, we have been able to engineer finite spin chains hosting spin waves [1] as well as the beginnings of a quantum phase transition at a critical magnetic field [2]. In a more recent experiment, we have engineered spin structures that are frustrated by design, exhibiting a spin spiral that can snap between different configurations. Unfortunately, the maximum size of assembled structures is often limited due to e.g. crystal impurity and crystal strain. In this talk, I will present a way to mitigate these limitations and show recent advances in sample preparation that will allow us to build much larger spin structures [3].

[1] A. Spinelli et al., Nature Matererials 13 (2014) 782
[2] R. Toskovic et al., Nature Physics 12 (2016) 656
[3] J. Gobeil et al., Surface Science 679 (2019) 202

O 99.2 Fri 11:00 H24

Exploring magnetic frustration in atomically engineered closed chains — •Jeremie Gobeil, David Coffey, Shang-Jen Wang, and Alexander F. Otte — Department of Quantum Nanoscience, Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands

Modelling quantum systems with a large number of degrees of freedom can be a daunting task from a computational standpoint. Scanning Tunneling Microscopy (STM) offers an alternative path by enabling atom-by-atom engineering and probing of such systems. Spin-Polarized STM (SP-STM) can provide direct insight into a system's spin configuration, while at the same time providing a tunable interaction parameter. This enables the study of frustrated spin systems, which pose a particular modelling challenge as they are governed by a delicate balance of competing interactions.

Here we present the study of such a frustrated spin system, consisting in closed chains of single iron atoms assembled on a single nitride layer grown on $Cu_3Au(100)$. As in the similar Cu_2N system, the nitride layer provides a uniaxial framework with different ferromagnetic and antiferromagnetic interatomic couplings depending on the relative position on the lattice. This allows us to assemble closed loop chains with an odd number of antiferromagnetic couplings, leading to frustration. We explore the role of an external magnetic field, interatomic exchange, as well as the exchange interaction with the spin-polarized tip in the stabilization of the resulting spin configuration.

O 99.3 Fri 11:15 H24

Revealing spin states in Co-salophene chains grown on $GdAu_2$ — •Maciej Bazarnik[1,2], Micha Elsebach[1], Emil Sierda[1,2], Maxim Ilyn[3], Jan Dreiser[4], Jens Brede[3], and Roland Wiesendanger[1] — [1]Department of Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany — [2]Institute of Physics, Poznan University of Technology, Piotrowo 3, 60-965 Poznan, Poland — [3]Centro de Física de Materiales, P° Manuel de Lardizabal 5, Donostia - San Sebastián, E-20018 Spain — [4]Swiss Light Source, Paul Scherrer Institut (PSI), CH-5232 Villigen, Switzerland

Lately, a polymerization of well-aligned organic nanowires was presented on a magnetic $GdAu_2$ surface alloy [1]. Apart from growing graphene on, i.e., a Ni surface, this was the first successful approach to a surface catalyzed reaction on a magnetic substrate. Such a ferromagnetic substrate in combination with magnetic molecules offers a very interesting interface for spintronic applications.

Here, we will present the growth behaviour of Co-salophene oligomers on the $GdAu_2$ surface alloy prepared on a Au(111) substrate. By combining spin-polarized scanning tunneling microscopy and X-ray magnetic circular dichroism we have revealed the evolution of the spin-* state residing on the Co-centers of the salophene molecules upon adsorption and thermally activated Ullmann coupling.

[1] M. Abadia et al. ACS Nano, 2017, 11 (12), pp 12392-12401

O 99.4 Fri 11:30 H24

Noncollinear spin density of an adatom on a magnetic surface — •Soumyajyoti Haldar and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, 24098, Kiel, Germany

Today, noncollinear spin structures at surfaces and interfaces receive great attention due to potential applications in spintronic devices. In such magnetic structures, the spin direction changes from atom to atom. Besides this inter-atomic noncollinear magnetism, there is also intra-atomic noncollinear magnetism in which the spin direction varies for different orbitals of an atom [1]. It can occur due to spin-orbit coupling or due to a noncollinear spin structure.

Here, we demonstrate that intra-atomic noncollinear magnetism can occur for adatoms on a magnetic surface with a noncollinear spin structure [2]. As an example, we study Co and Ir adatoms on Mn/W(110) using density functional theory. We find that the canted spin structure of the Mn surface layer is encoded into different orbitals of the adatoms. Our conclusions apply in general to adatoms on surfaces with a noncollinear magnetic structure e.g. spin spirals, skyrmions or domain walls and explain recent experimental results of spin-polarized scanning tunneling microscopy experiments [3].

[1] L. Nordström *et al.*, Phys. Rev. Lett. **76**, 4420 (1996)
[2] S. Haldar and S. Heinze, arXiv:1811.00865 (2018)
[3] D. Serrate *et al.*, Phys. Rev. B **93**, 125424 (2016)

O 99.5 Fri 11:45 H24

Interplay of spin-orbit and exchange interaction in ultrathin Ni films on W(110) — •Pascal Jona Grenz[1], Philipp Eickholt[1], Koji Miyamoto[2], Eike Schwier[2], Taichi Okuda[2], and Markus Donath[1] — [1]Institute of Physics, Westfälische-Wilhelms-

Universität Münster, Germany — [2]Hiroshima Synchrotron Radiation Center, Japan

Ferromagnetic adsorbates on W(110) are prototypical systems for studying the influence of spin-orbit and exchange interaction on electronic states. We investigated ultrathin Ni films on W(110) with spin- and angle-resolved photoemission with particular emphasis on (i) the influence of the Ni adsorbates on the Dirac-cone-like surface state of W(110), (ii) the spin dependence of electronic states at the interface between Ni and W, and (iii) the appearance of ferromagnetic order in the Ni overlayer. We will discuss our results in relation to similar systems reported in literature, Fe/W(110) and Co/W(110) [1,2].

[1] K. Honma *et al.*, Phys. Rev. Lett. **115**, 266401 (2015).

[2] P. Moras *et al.*, Phys. Rev. B **91**, 195410 (2015).

O 99.6 Fri 12:00 H24

Spin-dependent electron reflection at W(110) — •Christoph Angrick[1], Jürgen Braun[2], Hubert Ebert[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, Germany

The knowledge of the occupied, spin-dependent electronic structure of surfaces offers insights into spin phenomena and their possible use in spintronic devices. This knowledge can be obtained by photoemission techniques with subsequent spin-polarization analysis of the photoelectrons. The spin-polarization analysis relies on spin-dependent electron scattering and can be used in single- and multichannel modes [1,2,3,4].

Due to its strong spin-orbit coupling the W(110) surface is a promising candidate for the use as a scattering target in a spin-polarization analyzer. Therefore, the spin-dependent electron reflectivity of the W(110) surface was experimentally investigated for a wide range of incident electron energies and polar angles and compared with calculations. Two possible working points for spin-polarization analysis with a reversed sign in the Sherman function were found. The characteristics of the working points are discussed in view of an implementation in a single- and multichannel spin-polarization analyzer.

[1] Winkelmann *et al.*, Rev. Sci. Instrum. **79**, 083303 (2008).

[2] Okuda *et al.*, Rev. Sci. Instrum. **79**, 123117 (2008).

[3] Kolbe *et al.*, Phys. Rev. Lett. **107**, 207601 (2011).

[4] Tusche *et al.*, Appl. Phys. Lett. **99**, 032505 (2011).

O 99.7 Fri 12:15 H24

Investigation of superconductivity in spin chains on Re(0001) — •Lucas Schneider, Manuel Steinbrecher, Levente Rósza, Thore Posske, Jens Wiebe, and Roland Wiesendanger — Department of Physics, Hamburg University, 20355 Hamburg, Germany

Chains of magnetic atoms on high-Z s-wave superconductors can exhibit topological superconductivity and therefore host Majorana bound states at their ends [1, 2]. Most previous experimental work focused on self-assembled systems [3-4] where a change of the composition along the chain is difficult to achieve. In this study, we use the superconducting Re substrate which enables scanning tunneling microscope-tip induced assembly of chains that show indications for topological superconductivity [5]. This technique allows us to perfectly control the geometric properties and chemical composition of the chains. We evaporate different $3d$ transition metal adatoms as building blocks, assemble various linear chains and investigate their in-gap states. In particular, we studied the transition between magnetic and nonmagnetic regions in composite chains.

We acknowledge funding by the ERC via the Advanced Grant ADMIRE (No. 786020).

[1] Klinovaja *et al.*, PRL **111**, 186805 (2013). [2] J. Li *et al.* PRB **90**, 235433 (2014). [3] S. Nadj-Perge *et al.*, Science **346**, 6209 (2014). [4] M. Ruby *et al.*, Nano Letters **17**, 4473, (2017). [5] H. Kim *et al.*, Science Advances **4**, eaar5251 (2018).

O 99.8 Fri 12:30 H24

Thin film formation and processes in organic diradicals — •Tobias Junghöfer[1], Nolan Gallagher[2], Andrzej Rajca[2], and Maria Benedetta Casu[1] — [1]Eberhard Karls Universität Tübingen, Institut für Physikalische und Theoretische Chemie, 72076 Tübingen, Germany — [2]Department of Chemistry, University of Nebraska, Lincoln, Nebraska 68588-0304, USA

Organic radical thin films are of great interest for organic electronics such as spin filtering devices, data storage devices, and as quantum bits for quantum computing devices. The investigated diradicals possess two coupled spins with a combined magnetic moment (S = 1) which is of interest for novel applications in spintronics. In our work, we investigate chemically stable diradicals, deposited via organic molecular beam deposition (OMDB) in ultra-high vacuum. For our experiments, we use soft X-ray techniques, such as X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy, as well as atomic force microscopy (AFM). We demonstrate that we are able to deposit thin films of intact diradicals. We investigate their film formation properties and stability towards different environments.

O 99.9 Fri 12:45 H24

Optical and spin-orbit induced spin orientation of photoelectrons in the soft X-ray range — •Dmitry Vasilyev, Katerina Medjanik, Sergey Babenkov, Martin Ellguth, Gerd Schönhense, and Hans-Joachim Elmers — Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany

Angular- or k-resolved photoelectron spectroscopy in the soft X-ray range gives access to the bulk electronic structure of materials. Time-of-flight momentum microscopy with parallel spin detection extends this information to the spin degree of freedom. We choose tungsten as a paramagnetic model system in order to exclude any initial-state spin polarization from exchange-split bands. By measurement of four independent photoemission intensities for two opposite spin directions and opposite light helicity, we distinguish between spin polarization contributions of optical spin-orientation by circularly polarized X-rays (Fano component) and a second contribution with polarization direction perpendicular to the scattering plane. The latter phenomenon has been observed for surface states and is usually attributed to the surface-related inversion symmetry breaking. In the case of soft X-ray radiation, only inversion symmetric bulk states of tungsten are probed. Their finite perpendicular spin polarization thus represents a novel phenomenon originating from the spin-dependent interference of final state partial waves.

O 100: Overview Talk: Jürgen Behm

Time: Friday 13:15–14:00 Location: H15

Invited Talk O 100.1 Fri 13:15 H15

From UHV to Electrochemistry - Recent Developments — •R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Driven by the rapidly increasing role and importance of electrochemical Energy Technologies, e.g., in fuel cells, photovoltaics or batteries, electro-chemistry has emerged again as a highly active and rapidly growing field. The fundamental understanding of electrochemical processes is hampered, however, by the complex reaction conditions and the lack of established spectroscopic techniques. Similar to previous approaches in Heterogeneous Catalysis, Surface Science type model studies, both experimental and theoretical, have the potential to significantly contribute to a molecular-scale understanding of electrochemical and electrocatalytic reactions. These may reach from pure UHV studies on the chemical interaction between electrode and electrolyte via *ex situ* sample preparation and surface characterization under UHV conditions before / after exposure to electrochemical reaction conditions, which involves a controlled sample transfer between UHV and electrochemical cell, to finally *in situ* spectroscopic studies.

In the present talk I want to illustrate the potential of such kind of studies, using simple electrocatalytic reactions such as O_2 reduction or CO oxidation as example, but also other electrochemical processes. I will point out the close correlations and the validity of similar microscopic concepts for the description of reactions at the solid|gas and the solid|liquid interface, but also underline key differences. Finally, the importance of combined experimental and theoretical studies is demonstrated.