Surface Science Division
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

(Lecture rooms S054, S051, S052, S053, H24, H4, and H6; Poster A and E)

Overview, Invited, and Topical Talks

O 1.1	Mon	9:30–10:15	S054	**From surfaces and molecules to interfaces and hybrid materials: Theoretical spectroscopy of low-dimensional systems** — •Claudia Draxl
O 2.1	Mon	10:30–11:00	S054	**Hybrid plasmonic-photonic resonances for emitter control** — •Femius Koenderink
O 3.1	Mon	10:30–11:00	S051	**On growth and interaction phenomena of heteromolecular adsorbates on metal surfaces** — •Christian Kumpf
O 3.2	Mon	11:00–11:30	S051	**Surface Morphology from First-Principles: Thermodynamics and Kinetics** — •Karsten Reuter
O 3.3	Mon	11:30–12:00	S051	**Simulations of Surfaces and Interfaces Using High-Dimensional Neural Network Potentials** — •Jörg Behler
O 3.4	Mon	12:00–12:30	S051	**Morphology and growth of organic molecules at structured surfaces** — •Sabine H.L. Klapp, Nicola Kleppmann
O 3.5	Mon	12:30–13:00	S051	**Interaction of alcohols and water with carbonate surfaces** — •Angelika Kühnle, Christoph Marutschke, Felix Kling, Dirk Lautner, Ralf Bechstein, Peter Spijker, John Tracey, Ville Loukonen, Adam Foster
O 6.1	Mon	12:00–12:30	S053	**The surface science of friction: How molecular films affect sliding and plowing** — •Roland Bennewitz
O 7.5	Mon	11:30–12:00	H24	**Direct view on non-equilibrium carriers in graphene with time-resolved ARPES** — •Isabella Gierz
O 8.3	Mon	11:00–11:30	H4	**Momentum Microscopy with Time-of-Flight Analysis and Spin Filtering: Direct Imaging of k-Space Objects and Spin Textures** — •Gerd Schönhense
O 11.1	Mon	15:00–15:30	S054	**Principles of plasmonic imaging** — •Angela Demetriadou, Alexei Kornyshev
O 13.1	Mon	15:00–15:30	S052	**Excitations and dynamics of non-collinear magnetization states in tailored adatom arrays** — •Jens Wiebe
O 14.6	Mon	16:15–16:45	S053	**In-situ Studies of the Reactivity of Pt Model Catalysts: from Flat Surfaces to Nanoparticles** — •Christian Papp
O 15.4	Mon	15:45–16:15	H24	**Exploring chemical properties of surfaces by means of Atomic Force Microscopy** — •Pavel Jelinek
O 27.1	Tue	9:30–10:15	S054	**The Emergence of Covalent On-Surface Polymerization** — •Leonhard Grill
O 28.1	Tue	10:30–11:00	S054	**Unravelling the structural and electronic properties of organic/metal interfaces with photoemission tomography** — •Peter Puschnig
O 29.1	Tue	10:30–11:00	S051	**Toward single atom qubits on a surface: Pump-probe spectroscopy and electrically-driven spin resonance** — •William Paul
O 30.3	Tue	11:00–11:30	S052	**Taking Nanoscience to the Edge – The Different Appearances of One-Dimensional Physics** — •Jörg Schäfer
O 37.1	Tue	14:00–14:30	S054	**Metal Complexation of Sulfur on Coinage Metal Surfaces** — •Patricia Thiel, Holly Walen, Yousoo Kim, Junepyo Oh, Hyun Jin Yang, Da-Jiang Liu
O 41.1	Tue	14:00–14:30	H24	**Topological semimetals and chiral transport in inversion asymmetric systems** — •Shuichi Murakami

O 50.1	Wed	9:30–10:15	S054	**Shedding light on internal interfaces** — •Ulrich Höfer
O 51.1	Wed	10:30–11:00	S054	**Energy level alignment mechanisms at hybrid inorganic/organic semiconductor interfaces** — •Norbert Koch
O 53.1	Wed	10:30–11:00	S052	**Insights into Oxygen Evolution Electrocatalysis on Perovskites** — •Thomas J. Schmidt
O 53.2	Wed	11:00–11:30	S052	**Using redox agents to enhance the performance of lithium-air batteries and lithium recycling** — •Nuria Garcia-Araez
O 53.3	Wed	11:30–12:00	S052	**Probing the Femtosecond Dynamics of the Hydrogen Evolution Reaction on Gold** — •R. Kramer Campen, Francois Lapointe, Yujin Tong
O 53.4	Wed	12:15–12:45	S052	**The Electrochemical interface - at the atomic scale** — •Jan Rossmeisl
O 53.5	Wed	12:45–13:15	S052	**CO2 Electroreduction over Cu and Au Nanostructured Catalysts: Size, Oxidation State and Interparticle Distance Effects** — Hemma Mistry, Rulle Reske, Farzad Behafarid, Ana Sofia Varela, Peter Strasser, •Beatriz Roldan Cuenya
O 58.5	Wed	16:00–16:30	S054	**Thin Films of Metal-Organic Frameworks: Functional, photoswitchable coatings and unique model systems** — •Lars Heinke
O 60.1	Wed	15:00–15:30	S052	**First-principles photo-electrocatalysis beyond the computational hydrogen electrode** — •Harald Oberhofer
O 62.1	Wed	15:00–15:30	H24	**Topological semimetal phases in strained HgTe-based alloys** — Tomáš Rauch, Steven Achilles, •Jürgen Henk, Ingrid Mertig
O 62.2	Wed	15:30–16:00	H24	**Topological surface Fermi arcs and the chiral anomaly in Weyl semimetal materials** — •Binghai Yan
O 63.1	Wed	15:00–15:30	H4	**Spin-orbit coupling, magnetic perturbations, and competing trends in topological insulators** — •Matthias Bode
O 63.2	Wed	15:30–16:00	H4	**Conductance and shot noise spectroscopy of single magnetic atoms and molecules** — •Alexander Weismann
O 63.3	Wed	16:00–16:30	H4	**Manipulating spins in single molecules on a superconductor** — •Benjamin W. Heinrich
O 75.1	Thu	9:30–10:15	S054	**Ternary oxides with the perovskite structure exhibit an intriguingly rich variety in their physical and chemical properties.** — •Ulrike Diebold
O 76.1	Thu	10:30–11:00	S054	**Spin- and Pseudospin-Polarized Excited States in bulk WSe_2** — Roman Bertoni, Christopher Nicholson, Lutz Waldecker, Michele Puppin, Claude Monney, Cephise Cacho, Hannes Huebener, Umberto De Giovannini, Angel Rubio, Martin Wolf, •Ralph Ernstorfer
O 77.1	Thu	10:30–11:00	S051	**The first single atom magnet** — •Fabio Donati, Stefano Rusponi, Sebastian Stepanow, Christan Wäckerlin, Aparajita Singha, Luca Persichetti, Romana Baltic, Katharina Diller, Edgar Fernandes, François Patthey, Jan Dreiser, Željko Šljivančanin, Kurt Kummer, Corneliu Nistor, Pietro Gambardella, Harald Brune
O 77.2	Thu	11:00–11:30	S051	**When Electron Acceptors Donate Charge: Molecular Orbitals vs Hybrid Bands at Inorganic/Organic Interfaces** — •Oliver T. Hofmann, Patrick Rinke, Matthias Scheffler, Georg Heimel
O 77.3	Thu	11:30–12:00	S051	**Direct observation of H-bond dynamics using scanning tunneling microscopy** — •Takashi Kumagai
O 77.4	Thu	12:00–12:30	S051	**Visualizing topological states of matter and their interaction with perturbations using local probes** — •Paolo Sessi
O 77.5	Thu	12:30–13:00	S051	**Surface Chemistry of Oxygen and Water on Anatase TiO_2 (101)** — •Martin Setvin, Ulrich Aschauer, Jan Hulva, Michael Schmid, Annabella Selloni, Ulrike Diebold
O 80.1	Thu	10:30–11:00	H24	**Transport phenomena in broken-symmetry metals: Geometry, topology, and beyond** — •Ivo Souza
O 80.2	Thu	11:00–11:30	H24	**Dirac Fermions in Antiferromagnetic Semimetal** — •Peizhe Tang, Quan Zhou, Gang Xu, Shou-Cheng Zhang
O 81.1	Thu	10:30–11:00	H4	**Imaging orbitals and defects in superconducting FeSe/$SrTiO_3$** — •Jennifer Hoffman, Dennis Huang, Tatiana Webb, Shiang Feng, Can-Li Song, Cui-Zu Chang, Jagadeesh Moodera, Efthimios Kaxiras
O 84.1	Thu	15:00–15:30	S054	**Radio frequency STM on molecular resonators** — •Stefan Müllegger
O 85.1	Thu	15:00–15:30	S051	**Electrostatic Design of Organic Materials and Hybrid Interfaces** — •Egbert Zojer
O 87.3	Thu	15:30–16:00	S053	**Heteroatom-doped Molecular Nanostructures on Surfaces** — •Sabine Maier

O 89.5	Thu	16:00–16:30	H4	**The growth and decay of oxide quasicrystals** — •Stefan Förster, Jan Ingo Flege, Eva Maria Zollner, Florian Schumann, Klaus Meinel, Jens Falta, Wolf Widdra
O 93.1	Fri	9:30–10:15	S054	**New Science Opportunities with X-Ray Free-Electron Lasers** — •Wilfried Wurth
O 94.1	Fri	10:30–11:00	S054	**Time-resolved electron microscopy: probing ultrafast processes at the nanoscale** — •Sascha Schäfer
O 101.1	Fri	13:15–14:00	S054	**Ionic liquid surface science** — •Hans-Peter Steinrück

Invited talks of the joint symposium SYTI

See SYTI for the full program of the symposium.

SYTI 1.1	Wed	9:30–10:10	H1	**Topological insulators and topological superconductors** — •Shoucheng Zhang
SYTI 1.2	Wed	10:10–10:50	H1	**Three-dimensional topological insulators and superconductors** — •Yoichi Ando
SYTI 1.3	Wed	10:50–11:30	H1	**Interplay of magnetic and electronic states in pyrochlore iridates** — •Leon Balents
SYTI 1.4	Wed	11:40–12:20	H1	**Magnetic imaging of edge states** — •Kathryn Moler
SYTI 1.5	Wed	12:20–13:00	H1	**Sub-nm wide edge states at the dark side of a weak topological insulator** — •Markus Morgenstern

Invited talks of the joint symposium SYQS

See SYQS for the full program of the symposium.

SYQS 1.1	Wed	15:00–15:30	H1	**Magnonic macroscopic quantum states and supercurrents** — •Burkard Hillebrands, Dmytro A. Bozhko, Alexander A. Serga
SYQS 1.2	Wed	15:30–16:00	H1	**Elementary excitations of magnetic insulators and its heterostructures with metals** — •Gerrit Bauer
SYQS 1.3	Wed	16:00–16:30	H1	**Cavity Spintronics** — •Can-Ming Hu
SYQS 1.4	Wed	16:45–17:15	H1	**Hybrid Quantum Systems - Coupling Color Centers to Superconducting Cavities** — •Johannes Majer
SYQS 1.5	Wed	17:15–17:45	H1	**Quantum enhanced sensing with single spins in diamond** — •Fedor Jelezko

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Intrinsic Transport Coefficients and Momentum Space Berry Curvatures** — •Allan H MacDonald
SYES 1.2	Fri	10:00–10:30	H1	**Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems** — •Jairo Sinova
SYES 1.3	Fri	10:30–11:00	H1	**Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions** — •Ewelina Hankiewicz
SYES 1.4	Fri	11:15–11:45	H1	**Engineering Topological Quantum States: From 1D to 2D.** — •Jelena Klinovaja
SYES 1.5	Fri	11:45–12:15	H1	**Skyrmions – Topological magnetization solitons for future spintronics** — •Stefan Blügel

Sessions

O 1.1–1.1	Mon	9:30–10:15	S054	**Overview Talk: Claudia Draxl**
O 2.1–2.10	Mon	10:30–13:15	S054	**Plasmonics and Nanooptics I: Light-Matter Interaction**
O 3.1–3.5	Mon	10:30–13:00	S051	**Focus Session: Morphology Prediction at Interfaces**
O 4.1–4.8	Mon	10:30–12:30	S052	**Surface Magnetism: Atoms and Molecules**
O 5.1–5.6	Mon	10:30–12:00	S053	**Dynamics of Molecules on Surfaces**
O 6.1–6.4	Mon	12:00–13:15	S053	**Tribology**

O 7.1–7.11	Mon	10:30–13:30	H24	**Graphene I: Structure and Dynamics**
O 8.1–8.9	Mon	10:30–13:00	H4	**Surface State Spectroscopy I**
O 9.1–9.9	Mon	10:30–12:45	H6	**Nanostructures at Surfaces I**
O 10.1–10.11	Mon	9:30–13:00	H16	**Two-dimensional Materials**
O 11.1–11.11	Mon	15:00–18:00	S054	**Plasmonics and Nanooptics II: Microscopy**
O 12.1–12.14	Mon	15:00–18:30	S051	**Morphology Prediction at Interfaces**
O 13.1–13.9	Mon	15:00–17:30	S052	**Magnetic Surface Excitations**
O 14.1–14.11	Mon	15:00–18:00	S053	**Surface Chemical Dynamics**
O 15.1–15.13	Mon	15:00–18:30	H24	**STM/AFM: New Approaches**
O 16.1–16.12	Mon	15:00–18:00	H4	**Surface State Spectroscopy II**
O 17.1–17.13	Mon	15:00–18:15	H6	**Adsorption on Metal Surfaces**
O 18.1–18.10	Mon	17:00–19:30	Poster A	**Metallic Nanowires on Semiconductor Surfaces**
O 19.1–19.7	Mon	17:00–19:30	Poster A	**Semiconductor Substrates: Structure, Adsorption and Growth**
O 20.1–20.4	Mon	17:00–19:30	Poster A	**Tribology: Surfaces and Nanostructures**
O 21.1–21.8	Mon	18:15–20:30	Poster E	**Morphology Prediction at Interfaces: Theory meets Experiment**
O 22.1–22.17	Mon	18:15–20:30	Poster E	**Organic-Inorganic Hybrid Systems and Organic Films**
O 23.1–23.22	Mon	18:15–20:30	Poster E	**Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy**
O 24.1–24.11	Mon	18:15–20:30	Poster E	**Plasmonics and Nanooptics: Fabrication, Characterization and Applications**
O 25.1–25.6	Mon	18:15–20:30	Poster E	**Oxide and Insulator Surfaces: Structure and Growth**
O 26.1–26.6	Mon	18:15–20:30	Poster E	**Oxides and Insulator Surfaces: Adsorption**
O 27.1–27.1	Tue	9:30–10:15	S054	**Overview Talk: Leonhard Grill**
O 28.1–28.9	Tue	10:30–13:00	S054	**Organic-Inorganic Systems I: PTCDA**
O 29.1–29.11	Tue	10:30–13:30	S051	**Topology- and Symmetry-Protected Materials**
O 30.1–30.10	Tue	10:30–13:15	S052	**1D Metal Wires on Semiconductors I**
O 31.1–31.10	Tue	10:30–13:00	S053	**Heterogeneous Catalysis: Theory**
O 32.1–32.10	Tue	10:30–13:00	H24	**2D Materials I: Structure and Electronic Properties**
O 33.1–33.12	Tue	10:30–13:30	H4	**Photonics and Nanooptics I: Infrared Spectroscopy**
O 34.1–34.8	Tue	10:30–12:30	H6	**Nanostructures at Surfaces II**
O 35.1–35.12	Tue	9:30–13:15	H10	**Ultrafast Phenomena I**
O 36.1–36.4	Tue	13:30–15:30	H11	**Gaede Prize Talks**
O 37.1–37.7	Tue	14:00–16:00	S054	**Nanostructures at Surfaces III**
O 38.1–38.8	Tue	14:00–16:00	S051	**Spintronics**
O 39.1–39.8	Tue	14:00–16:00	S052	**1D Metal Wires on Semiconductors II**
O 40.1–40.8	Tue	14:00–16:00	S053	**Heterogeneous Catalysis: Experiment**
O 41.1–41.7	Tue	14:00–16:00	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport I**
O 42.1–42.8	Tue	14:00–16:00	H4	**Plasmonics and Nanooptics III: Infrared Microscopy**
O 43.1–43.8	Tue	14:00–16:00	H6	**Oxides and Insulators: Adsorption I**
O 44.1–44.12	Tue	18:15–20:30	Poster E	**Graphene: Electronic Properties, Structure and Substrate Interaction**
O 45.1–45.11	Tue	18:15–20:30	Poster E	**Graphene: Adsorption, Intercalation and Doping**
O 46.1–46.12	Tue	18:15–20:30	Poster E	**2D Materials beyond Graphene: TMDCs, Slicene and Relatives**
O 47.1–47.14	Tue	18:15–20:30	Poster E	**Electronic Structure of Surfaces: Spectroscopy, Surface States**
O 48.1–48.10	Tue	18:15–20:30	Poster E	**Electronic Structure: Surface Magnetism and Spin Phenomena**
O 49.1–49.13	Tue	18:15–20:30	Poster E	**Metal Substrates: Structure, Adsorption and Growth**
O 50.1–50.1	Wed	9:30–10:15	S054	**Overview Talk: Ulrich Höfer**
O 51.1–51.9	Wed	10:30–13:00	S054	**Organic-Inorganic Systems II: Energy Level Alignment**
O 52.1–52.11	Wed	10:30–13:15	S051	**Photonics and Nanooptics II: Nonlinear Response**
O 53.1–53.5	Wed	10:30–13:15	S052	**Focus Session: Electrocatalytic Energy Harvesting and Conversion**
O 54.1–54.10	Wed	10:30–13:00	S053	**2D Materials II: Growth**
O 55.1–55.10	Wed	10:30–13:00	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport II**
O 56.1–56.8	Wed	10:30–12:30	H4	**Nanostructures: Dots, Particles and Clusters**
O 57.1–57.9	Wed	9:30–13:00	H16	**Focus Session: Many-body effects in two-dimensional materials**

O 58.1–58.11	Wed	15:00–18:00	S054	**Organic-Inorganic Systems III: Metal-Organics**
O 59.1–59.13	Wed	15:00–18:15	S051	**Photonics and Nanooptics III: Fabrication and Characterization**
O 60.1–60.12	Wed	15:00–18:15	S052	**Chemistry at Solid/Liquid Interfaces**
O 61.1–61.12	Wed	15:00–18:00	S053	**Graphene II: Adsorption, Intercalation and Doping**
O 62.1–62.12	Wed	15:00–18:30	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport III**
O 63.1–63.5	Wed	15:00–17:00	H4	**Scanning Probe Microscopy and Spin Phenomena**
O 64.1–64.10	Wed	15:00–17:30	H6	**Oxides and Interfaces: Adsorption II**
O 65.1–65.12	Wed	14:45–18:30	H2	**Organic Photovoltaics and Electronics**
O 66.1–66.7	Wed	18:15–20:30	Poster A	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport**
O 67.1–67.5	Wed	18:15–20:30	Poster A	**Theory: General**
O 68.1–68.14	Wed	18:15–20:30	Poster A	**Nanostructures at Surfaces: 1D, 2D Structures and Networks**
O 69.1–69.12	Wed	18:15–20:30	Poster A	**Nanostructures at Surfaces: Dots, Particles, Clusters**
O 70.1–70.8	Wed	18:15–20:30	Poster A	**Nanostructures at Surfaces: Other Aspects**
O 71.1–71.19	Wed	18:15–20:30	Poster A	**Scanning Probe Techniques and New Experimental Methods**
O 72.1–72.10	Wed	18:15–20:30	Poster A	**Solid-Liquid Interfaces: Reactions and Electrochemistry**
O 73.1–73.17	Wed	18:15–20:30	Poster A	**Surface Dynamics: Reactions and Elementary Processes**
O 74.1–74.7	Wed	18:15–20:30	Poster A	**Ultrafast Electron and Spin Dynamics at Interfaces**
O 75.1–75.1	Thu	9:30–10:15	S054	**Overview Talk: Ulrike Diebold**
O 76.1–76.11	Thu	10:30–13:30	S054	**2D Materials beyond Graphene: Dynamics and Excitation**
O 77.1–77.5	Thu	10:30–13:00	S051	**Gerhard Ertl Young Investigator Award**
O 78.1–78.10	Thu	10:30–13:00	S052	**Nanostructures at Surfaces IV: Various Aspects**
O 79.1–79.9	Thu	10:30–12:45	S053	**Graphene III: Electronic Properties**
O 80.1–80.9	Thu	10:30–13:15	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV**
O 81.1–81.11	Thu	10:30–13:30	H4	**Oxides and Insulator Surfaces I**
O 82.1–82.10	Thu	10:30–13:00	H6	**Structure of Solid/Liquid Interfaces I**
O 83.1–83.13	Thu	9:30–13:15	H17	**Heterostructures and Interfaces**
O 84.1–84.12	Thu	15:00–18:15	S054	**Scanning Probe Techniques: Method Developments**
O 85.1–85.11	Thu	15:00–18:00	S051	**Organic-Inorganic Systems IV: Electronic Structure**
O 86.1–86.12	Thu	15:00–18:00	S052	**Ultrafast Surface Dynamics I**
O 87.1–87.12	Thu	15:00–18:15	S053	**Metal Substrates: Structure, Epitaxy and Growth**
O 88.1–88.13	Thu	15:00–18:15	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport V**
O 89.1–89.13	Thu	15:00–18:30	H4	**Oxides and Insulator Surfaces II**
O 90.1–90.8	Thu	14:45–17:15	H10	**Topological Insulators I**
O 91	Thu	19:00–19:30	H1	**Annual General Meeting of the Surface Science Division**
O 92	Thu	19:30–20:30	H1	**Post-Deadline Session**
O 93.1–93.1	Fri	9:30–10:15	S054	**Overview Talk: Wilfried Wurth**
O 94.1–94.6	Fri	10:30–12:15	S054	**Ultrafast Surface Dynamics II**
O 95.1–95.10	Fri	10:30–13:00	S051	**Graphene IV: Electronic Properties and Structure**
O 96.1–96.10	Fri	10:30–13:00	S052	**Structure of Solid/Liquid Interfaces II**
O 97.1–97.8	Fri	10:30–12:30	S053	**Nanostructured Surfaces and Thin Films**
O 98.1–98.11	Fri	10:30–13:15	H24	**Organic-Inorganic Systems V: Adsorption on Metals**
O 99.1–99.5	Fri	9:30–12:15	H1	**Symposium on Frontiers of Electronic Structure Theory: Focus on Topology and Transport**
O 100.1–100.8	Fri	9:30–12:00	H15	**Topological Insulators II**
O 101.1–101.1	Fri	13:15–14:00	S054	**Overview Talk: Hans-Peter Steinrück**

Annual General Meeting of the Surface Science Division

Time: Thursday 19:00–19:30 Audimax (H1)

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

Post–Deadline Session

Time: Thursday 19:30–20:30 Audimax (H1)

O 1: Overview Talk: Claudia Draxl

Time: Monday 9:30–10:15 Location: S054

Invited Talk O 1.1 Mon 9:30 S054
From surfaces and molecules to interfaces and hybrid materials: Theoretical spectroscopy of low-dimensional systems — •Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Germany — Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany

Ab initio spectroscopy is a powerful combination of quantum-based theories and computer simulations. It covers a wide range of theoretical and computational methods, which go beyond density-functional theory by incorporating many-body effects and interactions that show up in the excited state. This methodology not only allows for analyzing data obtained by experimental probes like photoemission, optical absorption, Raman, infrared, X-ray, and electron-loss spectroscopy, but also for shining light onto the underlying processes. These may be distinctively different depending on the nature and dimensionality of the material. Low-dimensional systems and interfaces challenge our theoretical concepts and numerical approaches. A series of selected examples – from surfaces and molecules to interfaces and organic-inorganic hybrid materials – will show how we can explore exciting new phenomena, where we are in our theoretical understanding, and what the major issues are that need to be tackled.

O 2: Plasmonics and Nanooptics I: Light-Matter Interaction

Time: Monday 10:30–13:15 Location: S054

Invited Talk O 2.1 Mon 10:30 S054
Hybrid plasmonic-photonic resonances for emitter control — •Femius Koenderink — Center for Nanophotonics, FOM Institute AMOLF, Amsterdam, The Netherlands

Plasmonic nanostructures match light to molecular length scales by hybridizing photons with charge density oscillations in noble metals. Plasmonics is pursued for many prospective uses ranging from sensing, spectroscopy, and microscopy, to the development of ultrabright single photon sources and broadband cavity QED for quantum information processing. I will report on our effort to use plasmonics to completely control when, into which direction, and with what polarization and wavefront single nanosources emit. I will particularly focus on Fourier-space polarimetry on single nano-antenna structures, as well as distributed periodic and quasiperiodic plasmonic structures for directional fluorescent, and lasing sources. Also, I will discuss the surprising physics of hybridizing plasmonics and dielectric nanophotonics. Recently we showed that, counter to conventional cavity perturbation theory, plasmonic structures can improve the quality factor of an already high-Q (exceeding 1 million) microtoroid. Finally, I will argue that hybrid plasmon-cavity structures can combine cavity Q-factors with plasmonic mode volumes.

O 2.2 Mon 11:00 S054
Coherent and periodic energy transfer between widely separated and cavity-coupled nanoantennas — Martin Aeschlimann[1], Tobias Brixner[2], Benjamin Frisch[1], Bert Hecht[3], Bernhard Huber[2], •Matthias Hensen[4], Christian Kramer[2], Enno Krauss[3], Thomas Löber[5], Walter Pfeiffer[4], Martin Piecuch[1], and Philip Thielen[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Department of Physical and Theoretical Chemistry, Würzburg University, 97074 Würzburg, Germany — [3]Experimental Physics 5, Würzburg University, 97074 Würzburg, Germany — [4]Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [5]Nano Structuring Center, TU Kaiserslautern, 67663 Kaiserslautern, Germany

We present a device that couples two widely separated ($d \approx 2\lambda_0$) nanoantennas via an extended plasmon mode in a metallic cavity of elliptical shape. As predicted by finite-difference time-domain simulations a coherent back and forth transfer of energy between the antennas is observed in experiments. Samples were made out of atomically-flat single crystalline gold plates and the temporal dynamics of plasmonic excitations was investigated by time-resolved photoelectron emission microscopy. The device depicts an all-plasmonic analogue of the quantum mechanical Tavis-Cummings model and it is particularly suited to study the interaction of deterministically positioned quantum systems coupled to the incorporated nanoantennas.

O 2.3 Mon 11:15 S054
Far-field interferometry of weak plasmonics scatterers — •Christian Dicken[1], Daniela Wolf[1], Thorsten Schumacher[1], Klas Lindfors[2], Harald Giessen[3], and Markus Lippitz[1] — [1]Institute of Experimental Physics III, University of Bayreuth, Germany — [2]Department of Chemistry, Nanooptics Group, University of Cologne, Germany — [3]Institute of Experimental Physics IV, University of Stuttgart, Germany

Low-loss noble metals like gold and silver are at the heart of plasmonics. Yet, many applications focus on metals with higher losses and less pronounced optical response. We discuss how a simple mirror and a dielectric spacer layer turn a transmission experiment into an interferometer. This scheme is used by us in a simple model to optimize the sensitivity to small changes of the optical response of weak scatteres. In particular, we present interferometrically detected magnetic hysteresis loops of sub-100nm nickel disks and compare the data with our model.

O 2.4 Mon 11:30 S054
Photoluminescence Enhancement by laterally ordered Ag/Alq$_3$:ZnPc/Ag Nanocavities — •Verena Kolb[1] and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Center of Applied Energy Research (ZAE Bayern), 97074 Würzburg

Plasmonic nanostructures provide a perfect possibility to tailor the photoluminescence (PL) of organic semiconductors. In this contribution we present PL investigations on silver nanoprism arrays prepared by shadow nanosphere lithography and resonantly coupled to the luminescence of ZnPc (zinc phthalocyanine) molecules. Confocal PL measurements revealed a strong increase of the fluorescence of ZnPc thin films deposited on top of the nanoprisms. Co-evaporation into an Alq$_3$ (tris(8-hydroxyquinoline)aluminum) matrix at low concentrations of 4% leads to further increase, which can be explained by the reduction of non-radiative processes caused by exciton-exciton-annihilation and quenching at metal/organic interface. Lateral structuring of the organic layer and capping by silver result in periodically ordered Ag/Alq$_3$:ZnPc/Ag hybrid structures with PL enhancement factors up to 700 after geometrical correction. Complementary FDTD simulations confirm the pronounced spectral overlap between the localized surface plasmon resonance and the highest PL mode and thus, are able to prove the enhancement to be of plasmonic origin.

O 2.5 Mon 11:45 S054
Optical rotation reversal and circular dichroism in resonantly and off-resonantly coupled plasmonic nanosystems — •Mario Hentschel[1,2], Vivan E. Ferry[3], A. Paul Alivisatos[1], and Harald Giessen[2] — [1]Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, United States — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [3]Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, United States

In a system consisting of two resonant L-shaped particles we show that the sign of the circular dichroism spectrum in a plasmonic system can be controllably changed through small geometric perturbations that change the energetic ordering of the hybridized modes [1]. This mechanism is distinct from geometrical changes that explicitly change the handedness of the system. Secondly, we investigate the role of resonant coupling in chiral plasmonic systems, and whether the formation of collective plasmonic modes in a handed assembly of metallic nanostructures is a necessary condition for a chiroptical response. We show in experiment and simulation that off-resonant coupling between spectrally detuned nanostructures arranged with structural chirality leads to a clear yet weak chiroptical response [2]. We interpret our results in the framework of scattering between the individual constituents that in turn leads to a chiroptical farfield response. [1] M. Hentschel et al., ACS Photonics 2, 1253 (2015) [2] V. E. Ferry, M. Hentschel, and A. Paul Alivisatos, Nano Lett. 15, DOI 10.1021/acs.nanolett.5b03970

O 2.6 Mon 12:00 S054

Enantiomorphic chiral near-fields in locally chiral plasmonic lattices — •Martin Schäferling, Xinghui Yin, Maxim Nesterov, Harald Giessen, and Thomas Weiss — 4th Physics Institute and Research Centers SCoPE and SimTech, University of Stuttgart, Germany

Chiral near-fields, which interact strongly with chiral molecules, can be obtained by illuminating geometrically chiral plasmonic nanostructures with circularly polarized light [1,2]. Fields with opposite handedness can be used to probe the chiroptical properties of chiral molecules with enhanced sensitivity. However, the field pairs generated by periodic arrangements of chiral nanostructures are, in general, not enantiomorphic. Additionally, such structures exhibit a chiroptical far-field response even in absence of chiral probe molecules. Both effects hamper the implementation of plasmonically enhanced chiroptical spectroscopy schemes.

In this contribution, we discuss periodic arrangements of simple achiral building blocks where the resulting superstructure is geometrically achiral, but still provides left- and right-handed geometrically chiral substructures. Due to their symmetry, such configurations provide enantiomorphic chiral near-fields, but no chiroptical far-field response. We show how to identify all such arrangements of plasmonic nanodiscs in a 4×4 unit cell that additionally provide C_4 symmetry and compare the simulated chiroptical near-field response of selected examples.

[1] Y. Tang and A. E. Cohen, Science **332**, 333 (2011).

[2] M. Schäferling et al., Phys. Rev. X **2**, 031010 (2012).

O 2.7 Mon 12:15 S054

Circular Dichroism Spectroscopy on Individual Plasmonic Nanoparticles — •Julian Karst[1], Nikolai Strohfeldt[1], Mario Hentschel[1], Harald Giessen[1], and Na Liu[2] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Max-Planck-Institute for Intelligent Systems, Stuttgart, Germany

Chirality is one of the most important basic principles of nature. We analyze the chiroptical response of single chiral plasmonic nanostructures. We utilize dark field circular dichroism spectroscopy to study the response of individual 3D chiral plasmonic Au-nanostructures. A customized spectroscopy setup for the visible spectral range is used. Transmission and scattering spectra are measured with a bright field and dark field spectroscopy setup, respectively. With large area ensembles of achiral and chiral plasmonic nanostructures we determine the influence of several optical components in the light path as well as the influence of fabrication defects. We show that individual chiral plasmonic oligomers in C$_1$ and C$_4$ configuration exhibit a mirror symmetry in the circular dichroism spectra for the right- and left-handed enantiomers. However, we see clear differences in the response of C$_1$-symmetric Au-nanostructures compared to the polarization conversion suppressing C$_4$-symmetric structures. The successful measurements of the chiroptical response of single chiral three dimensional plasmonic oligomers pave the way for studying more complex individual DNA based chiral plasmonic nanostructures.

O 2.8 Mon 12:30 S054

Device design from stacked metasurfaces by use of a modified S-Matrix formalism — •Jan Sperrhake, Christoph Menzel, and Thomas Pertsch — Institut für angewandte Physik, Abbe Center of Photonics, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

Artificial subwavelength structures called metamaterials (MM) are one of the most promising approaches in modern photonics for full control of light with respect to its polarization and spectral properties. By using MM made of complex shaped 3D elements almost arbitrary optical functionalities can be integrated into thin films. However, as the fabrication of 3D MM is usually difficult, complexity of the optical response might be achieved instead by choosing 2D metasurfaces (MS) and stacking them. In this contribution, we propose a method for efficiently treating and optimizing stacked complex homogeneous MS to create integrated, highly functional optical devices. A theoretical framework for fast numerical calculation is given by means of a modified scattering matrix formalism providing full information about phase, amplitude and polarization of the desired reflected and transmitted fields. As we will show with some examples this will pave the way towards simpler structures and easier fabrication, while maintaining and even increasing the range of accessible optical functionalities. A preprint of the paper is available at http://arxiv.org/abs/1511.09239.

O 2.9 Mon 12:45 S054

Efficiency analysis of a finite-difference modal method for the derivation of electromagnetic fields — •Izzatjon Allayarov, Martin Schäferling, Maxim Nesterov, and Thomas Weiss — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Accurate numerical derivation of electromagnetic fields is important for many questions such as modeling the enhanced spontaneous emission due to the Purcell effect. Finite element methods (FEM) offer high accuracy, but are slow and tedious to implement. For periodic systems, the Fourier modal method (FMM) is a fast and reliable alternative. However, the underlying Fourier basis cannot resolve high contrasts of the dielectric constant accurately, which is especially problematic when fields close to such interfaces should be calculated.

We present an implementation of a finite difference basis for modal methods (FDMM) [1], which can exactly model arbitrary steps in the dielectric constant. We compare the accuracy and the calculation time to standard FMM as well as to FEM. Our results indicate that the accuracy of the fields is higher for the FDMM compared to the FMM for comparable calculation times.

Additionally, we will discuss the possibility to combine this finite-difference basis with the coordinate transformation methods that have already been applied to the FMM [2]. This will allow for precise calculations of non-rectangular geometries using the FDMM.

[1] I. Semenikhin, and M. Zanuccoli, JOSA A **30**, 2531 (2013).

[2] T. Weiss et al., Opt. Express **17**, 8051 (2009).

O 2.10 Mon 13:00 S054

Analytical model for hybrid magnetoplasmonics — •Dominik Floess[1], Thomas Weiss[1], Sergei Tikhodeev[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]A. M. Prokhorov General Physical Institute, Russian Academy of Sciences, Moscow

In recent years, the hybrid plasmonic construction kit was expanded by magneto-optical materials, which offer magnetic tuning and non-reciprocal effects. By utilizing localized surface plasmons, the magneto-optical response of dielectric thin films can be resonantly amplified and spectrally tailored. While the experimental realization of such systems received considerable attention, so far there is no profound theoretical description that goes beyond numerical simulations. Here we present an intrisically non-reciprocal coupled oscillators model that reveals the underlying physics inside such systems and yields analytical expressions for the resonantly enhanced magneto-optical response. The predictions of the model are in good agreement with full numerical simulations of typical sample geometries as well as experiments. This includes modal dispersion, optical rotation and ellipticity.

O 3: Focus Session: Morphology Prediction at Interfaces

Time: Monday 10:30–13:00 Location: S051

Topical Talk O 3.1 Mon 10:30 S051

On growth and interaction phenomena of heteromolecular adsorbates on metal surfaces — •Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich GmbH, Jülich, Germany, and Jülich-Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

The properties of functional materials and electronic devices are often dominated by their surfaces and interfaces. This is particularly true for organic thin films and adsorbate systems as they are frequently used in the field of organic electronics. Molecular blends (i.e., heteromolecular layers containing at least two different types of molecules, usually charge donors und acceptors) are of particular interest in this context. We have investigated a number of heteromolecular model systems containing either PTCDA or NTCDA as acceptor molecules, and CuPc or SnPc as donors.

In this talk I will concentrate on monolayer films consisting of PTCDA and CuPc, which we have studied using a variety of experimental methods like LEEM, LEED, STM, NIXSW, ARPES, orbital tomography and STS. A comprehensive LEEM study enabled us to understand the complex binary phase diagram containing three different ordered heteromolecular structures with different stoichiometry, several regimes with coexisting phases and a 2D-lattice gas. We identified the density of the gas phase to be the crucial parameter determining the growth behavior of the ordered structures on the surface. Furthermore, I will discuss the interaction of the two types of molecules with the surface in terms both its geometric and electronic fingerprints.

Topical Talk O 3.2 Mon 11:00 S051

Surface Morphology from First-Principles: Thermodynamics and Kinetics — •Karsten Reuter — Technische Universität München

The structure of functionalized surfaces or surfaces exposed to realistic environments depends sensitively on the deposition conditions or gas-phase conditions. Detailed atomic-scale knowledge of this structure is often a prerequisite for further analysis and understanding. With experiment struggling to provide sufficient resolution, predictive-quality first-principles computational approaches assume a critical role in gaining this knowledge. Their task is then an efficient exploration of the vast configuration spaces, identifying (meta-)stable states and critical barriers on the high-dimensional potential energy surface.

While this task is thus simply summarized in one sentence, the words "efficient", "vast" and "high-dimensional" contained in it equally highlight the challenges faced in actually accomplishing this endeavour for anything but simple model systems. Knobs to turn are the way the algorithms navegate through configuration space, reduced-cost energy functions used for large-scale pre-screenings, or the use of coarse-grained lattice models. In this talk I will review our recent activities in this field, focusing on examples that are governed by both thermodynamic and kinetic factors.

Topical Talk O 3.3 Mon 11:30 S051

Simulations of Surfaces and Interfaces Using High-Dimensional Neural Network Potentials — •Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

In recent years a lot of progress has been made in the development of interatomic potentials based on machine learning techniques. These potentials are very efficient and thus allow to extend the length and time scales of molecular dynamics simulations significantly. Further, they are close to the accuracy of the underlying reference electronic structure methods and equally applicable to all types of bonding making them particularly useful for complex systems like interfaces. After a short overview about the available approaches, specifically the class of high-dimensional neural network potentials will be discussed. Several applications including water and solid-liquid interfaces will be presented to illustrate the advantages and current limitations of this method.

Topical Talk O 3.4 Mon 12:00 S051

Morphology and growth of organic molecules at structured surfaces — •Sabine H.L. Klapp and Nicola Kleppmann — Institut für Theoretische Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

We report about recent progress in modelling organic molecules at structured inorganic, particularly semiconductor surfaces on a coarse-grained level of description. We start by discussing multilayer growth of the organic molecule C60. Based on kinetic MC simulations we quantify this time-dependent process and extract a self-consistent set of energy parameters, which lead to excellent agreement with parallel, real-time x-ray measurements. We then proceed to the structure formation and dynamics of the strongly anisotropic molecule para-sexiphenyl (6P) at ZnO surfaces. To this end we propose a new, coarse-grained model which aims at representing heuristically the different electrostatic and steric interactions occuring at the charge-patterned surface ZnO(10-10). Corresponding MC simulations of the equilibrium behavior reveal indeed a complex interplay of the different contributions of this coarse-grained Hamiltonian. Finally, based on kMC simulations and a rate equation approach we explore the non-equilibrium surface growth of 6P at finite adsorption rates, revealing re-entrant effects, a critical adsorption rate and observables that are non monotonous with the adsorption rate. Our results form a basis for understanding and predicting collective orientational ordering during growth in hybrid material systems.

Topical Talk O 3.5 Mon 12:30 S051

Interaction of alcohols and water with carbonate surfaces — •Angelika Kühnle[1], Christoph Marutschke[1], Felix Kling[1], Dirk Lautner[1], Ralf Bechstein[1], Peter Spijker[2], John Tracey[2], Ville Loukonen[2], and Adam Foster[2] — [1]Universität Mainz — [2]Aalto University

Carbonate minerals are abundant in the earth's crust and constitute the inorganic phase in many bio-minerals created by nature. Understanding the formation and reactivity of carbonates in their natural environment requires elucidating the interaction of organic molecules with the mineral surface in the presence of water. We have studied the solid-liquid interface at the natural cleavage plane of the most common carbonates, i.e., calcite, magnesite and dolomite using high-resolution atomic-force microscopy (AFM) imaging and three-dimensional solvation layer mapping. Representing the simplest organic molecules, we have studied methanol, ethanol and their competition with water on the carbonate surfaces. In combination with molecular dynamics simulations we explain the observed solvation structures and provide evidence for stronger ethanol-calcite interaction as compared to water-calcite interaction.

We complement our liquid environment studies by an investigation in ultra-high vacuum (UHV). Thermal desorption spectroscopy obtained at sub-monolayer coverage confirms that ethanol is more strongly bound to calcite as compared to water. In combination with theoretical simulations we disclose atomic-scale details of the water-carbonate as well as the alcohol-carbonate interaction.

O 4: Surface Magnetism: Atoms and Molecules

Time: Monday 10:30–12:30 Location: S052

O 4.1 Mon 10:30 S052

Magnetic Hysteresis in Er trimers on Cu(111) — •Aparajita Singha[1], Fabio Donati[1], Christian Wäckerlin[1], Romana Baltic[1], Jan Dreiser[1,2], Marina Pivetta[1], Stefano Rusponi[1], and Harald Brune[1] — [1]École Polytechnique Fédérale de Lausanne, Switzerland — [2]Swiss Light Source, Paul Scherrer Institute, Switzerland

The aim to explore the ultimate density limit of magnetic information storage has triggered increasing interest in surface-supported magnetic nanostructures. Currently the smallest surface-adsorbed ferromagnet consists of only five Fe atoms with magnetic stability up to several hours at 0.3 K [1]. Here, we present evidence of magnetic hysteresis in rare earth Er clusters at 2.5 K starting from the size of three atoms. We combine x-ray magnetic circular dichroism, scanning tunneling microscopy and mean-field nucleation theory to determine the size-dependent magnetic properties of the Er clusters adsorbed on Cu(111). We observe that the magnetization of Er atoms [2] and dimers is oriented in-plane. In contrast, trimers and bigger clusters exhibit out-of-plane anisotropy and a butterfly-shaped magnetic hysteresis at 2.5 K. Their magnetization lifetime is larger than 120 s at 0.1 T.

[1] Khajetoorians et al., Science, 339, 55 (2013) [2] Donati et al., Phys. Rev. Lett., 113, 237201 (2014)

O 4.2 Mon 10:45 S052

Calibration of highly efficient FeO-based spin polarization detector — •Pika Gospodaric, Ewa Mlynczak, Markus Eschbach, Mathias Gehlmann, Sven Döring, Lukasz Plucinski, and Claus Michael Schneider — Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52425 Jülich, Germany

A recently developed FeO-based spin polarization detector (1) was adapted to a high-resolution hemispherical MBS A-1 electron analyzer to study the spin degree of freedom in the electronic band structure of spintronic materials with spin- and angle-resolved photoemission spectroscopy (spinARPES). The operation of the polarimeter is based on the exchange scattering of electrons from an oxidized Fe(100) film, which can be magnetized in four orthogonal in-plane directions. Our setup employs a 90° deflector, which allows probing one of the in-plane and the out-of-plane spin components. In this talk, performance calibration tests of the system using the Rashba spin-orbit split surface states of the single crystal Au(111) and various topological insulator thin films will be presented. At optimized scattering energy the asymmetry function reaches 30% and the reflectivity up to 10%, which results in a 20-40 times higher figure of merit compared to the conventional Mott spin detectors. Experiments were performed using an unpolarized noble-gas discharge lamp and a laser-based 6 eV photon source with light polarization control. The high energy and angular resolution of the spinARPES spectra clearly distinguishes the two spin polarized branches of the Au(111) surface state.

(1) M. Escher et al., e-J. Surf. Sci. Nanotech. Vol. 9 (2011)

O 4.3 Mon 11:00 S052

Electronic and magnetic properties of Au/Fe(001) bilayers epitaxially grown on MgO(001) — •Ewa Młyńczak^{1,2}, Pika Gospodarič^{1}, Markus Eschbach^{1}, Mathias Gehlmann^{1}, Sven Döring^{1}, Lukasz Plucinski^{1}, and Claus Michael Schneider^{1} — ^{1}Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52425 Jülich, Germany — ^{2}Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, al. Mickiewicza 30, 30-059 Kraków, Poland

The electronic band structure of ferromagnetic films is a basis for magnetotransport phenomena, which are important for future spintronics, such as tunneling anisotropic magnetoresistance or spin-orbit torque (SOT). In the context of SOT, it is especially interesting to study the electronic structure of the interface between a ferromagnet (characterized by high exchange coupling) and a heavy metal (known for high spin-orbit coupling). In this study, ultrathin Au layers were deposited onto Fe(001)/MgO(001) thin film using different preparation conditions. The Au growth was monitored by recording changes of the film resistance with the deposition time. A laboratory based high-resolution angle resolved photoemission spectroscopy was used to study the near-surface electronic band structure. Spin detection was performed using a highly efficient spin polarimeter (FERRUM). It was possible to observe the development of the electronic bands characteristic for Au, while still having experimental access to the band structure of the underlying Fe(001). The magnetic properties of the bilayers were determined by in-situ anisotropic magnetoresistance measurements.

O 4.4 Mon 11:15 S052

The fascinating versatility of wustite surfaces — •Silvia Gallego and Ivan D. Bernal-Villamil — Instituto de Ciencia de Materiales de Madrid, Madrid, Spain

Wustite (FeO) belongs to the magnetic transition metal monoxides series, a set of antiferromagnetic Mott insulators with a simple rock-salt structure. Among them, wustite is singular in its high content of Fe vacancies at ambient conditions, that introduce local polaronic charge distributions and alter the magnetization.

Mono- and bi-layer FeO has been grown and largely studied, but it reverts to Fe3O4 as the thickness increases, accompanied by a yet not solved 2x2 surface structure with unexpected magnetic features. Based on ab initio calculations, in this talk we will provide our solution for this 2x2 structure, explaining the evolution of FeO to Fe3O4, and the origin of the magnetism. Furthermore, we will show how surface processes are involved in the growth of unusually thick stoichiometric FeO films, that hold a 1x1 symmetry and robust bulk-like antiferromagnetic order.

O 4.5 Mon 11:30 S052

Theory of Inelastic Electron Tunneling through an Adatom: Perturbation Expansion around the Atomic Limit — •Jindrich Kolorenc — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

We investigate tunneling of electrons from an STM tip to a substrate through a magnetic adatom. We assume weak coupling between the tip and the adatom as well as between the adatom and the substrate, and we include these couplings only in the lowest order of the perturbation theory. We employ the Kramers–Heisenberg formula to evaluate the probabilities of coherent two-step processes that contribute to the tunneling current (for instance, an electron tunnels from the tip to the adatom and then continues from the adatom to the substrate). Our method is closely related to the cotunneling theory of Ref. [1], but it appears somewhat more straightforward and allows us to derive a relatively compact formula for the differential conductance. The steps appearing in the differential-conductance spectra are identified with excitations in the magnetic adatom that can be parametrized on the basis of first-principles calculations without resorting to an effective spin model. The method is straightforwardly applicable to cases with strong spin-orbital coupling (f electrons) where the spin is not a good quantum number.

[1] F. Delgado and J. Fernández-Rossier, Phys. Rev. B **84**, 045439 (2011)

O 4.6 Mon 11:45 S052

Investigation of the superconducting gap of nano-sized Pb-islands in high magnetic fields — •Steffen Rolf-Pissarczyk^{1,2}, Jacob Burgess^{1,2}, Shichao Yan^{1,2}, and Sebastian Loth^{1,2} — ^{1}Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — ^{2}Max Planck Institute for Solid State Research, Stuttgart, Germany

Superconductors change drastically their properties when they are confined in geometries with dimensions of the order or less than the London penetration depth or coherence length of the bulk material. To get experimental access to the effects of strong confinement we prepared small hexagonal Pb-islands with diameter of less than 50 nm and a uniform height of 7 atomic layers on Si(111) 7x7. The islands were formed by depositing Pb at low temperature and annealing at 300 K. We investigated the Pb-islands with scanning tunneling spectroscopy in magnetic fields up to 9 T and at 0.6 K temperature.

We found the critical magnetic field in such small islands to be several Tesla, which represents an enhancement greater than 50 compared to the bulk value. The critical field was directly measured and verified by the vanishing superconducting gap. By independently measuring the size of the superconducting gap and the critical magnetic field that quenches superconductivity we were able to correlate these two fundamental parameters. This correlations allows us to estimate the highest critical field expected for 7 atomic layer thin Pb-islands.

O 4.7 Mon 12:00 S052

Sensing Nanomagnets with an Atomically Assembled Quantum Spin Sensor — •Luigi Malavolti^{1,2}, Shichao Yan^{1,2}, Jacob Burgess^{1,2}, Steffen Rolf-Pissarczyk^{1,2}, and Sebastian Loth^{1,2} — ^{1}Max-Planck Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland — ^{2}Max-Planck Institut für Festkörperforschung, Hamburg, Deutschland

Quantum spin systems can be used for sensing the magnetic environment with unprecedented accuracy and sensitivity [1]. Atom manipulation in the scanning tunnelling microscope allows construction of the quantum sensor in close proximity to the objects or region of interest.

Here, we show that a quantum spin sensor consisting of three Fe atoms on a monolayer copper nitride surface [2] can be used to probe the magnetic state of nearby nanomagnet. We built a nanomagnet that show no net spin and switches spontaneously between two Néel states. By characterizing the dynamic magnetic behaviour of the sensor using a dynamic pump-probe technique [2,3] we were able to detect the state of the nanomagnet at distance up to 3nm. We also demonstrate that, by an appropriate tuning of the properties of our sensor, the non-local sensing is possible even without a direct access to the relaxation time of the sensor. This opens the way to non-locally detect the magnetic state of other magnetic objects such as single molecule magnets and local atomic conditions on surfaces.

[1] Damadian, R. Science 171(3976), 1151-1153 (1971).
[2] Yan, S., et al., Nat Nano 10(1), 40-45 January (2015).
[3] Loth, S., et al., Science 329(5999), 1628-1630 (2010).

O 4.8 Mon 12:15 S052

X-ray magnetic dichroism of small, size-selected FeV clusters on Cu(100) — •Fridtjof Kielgast^{1}, Torben Beeck^{1}, Ivan Baev^{1}, Deniza Chekrygina^{1}, Michael Martins^{1}, and Wilfried Wurth^{1,2} — ^{1}Physics Department, University of Hamburg — ^{2}DESY Photon Science, Hamburg

The electronic and magnetic properties of clusters tend to change strongly depending on size and composition of the clusters. This change is of great interest both in fundamental and applied research. Here we investigate clusters of 3d metal alloys produced by high energy sputtering. A magnetic field is used to separate the clusters depending on their mass-to-charge ratio. Pure Fe and V adatoms, $Fe_{2,3}$ and V_2 as well as V_1Fe_1 clusters, deposited onto a Cu(100) surface were studied using XMCD. The magnetic XMCD signal was obtained by switching an external magnetic field (±7 T) and scanning the $L_{2,3}$ edges with circular polarized light at the P04 beamline at PETRA III, DESY. To avoid fragmentation or implantation of the clusters into the substrate, the deposition was carried out by using a soft landing scheme. This work is supported by the DFG in the framework of the SFB 668.

O 5: Dynamics of Molecules on Surfaces

Time: Monday 10:30–12:00 Location: S053

O 5.1 Mon 10:30 S053

Electric field driven chemical reaction of single molecules by Scanning Tunneling Microscopy — •Tomasz Michnowicz[1], Bogdana Borca[1], Verena Schendel[1], Ivan Pentegov[1], Ulrike Kraft[1], Hagen Klauk[1], Peter Wahl[1,2], Uta Schlickum[1], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]University of St Andrews, School of Physics and Astronomy, KY16 9SS St Andrews, UK — [3]Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Scanning Tunneling Microscopy allows the manipulation of individual organic molecules by various kinds of stimuli, for example tunneling current, electric field or precise mechanical interaction. Here we present a study of chemical bond formation of individual organic molecules, tetracenothiophene (TCT), to the copper (111) surface by making use of the electric field present between tip and surface. Ramping the bias voltage, while positioning the tip apex precisely above the thiophene group, results in a change of the molecule's topographic appearance, which we attribute to the breaking of the thiophene group and a chemical bond formation to the copper surface atoms. The threshold voltage, that has to be overcome in order to trigger the reaction, depends linearly on the tip-molecule distance. This is a characteristic behaviour for electric field driven processes. In addition, we measured the single molecule's conductance of about 0.14 G_0 for molecules before reaction and 0.21 G_0 for molecules after reaction (G_0: quantum of conductance).

O 5.2 Mon 10:45 S053

Simultaneous AFM/STM study of chirality and on-surface chemistry of Dibenzo[7]helicene deposited on Ag(111) — •Oleksander Stetsovych[1], Martin Svec[1], Jaroslav Vacek[2], Jana Vacek-Chocholousova[2], Irena Stara[2], Andrej Jancarik[2], Jiri Rybacek[2], Pavel Jelinek[1], and Ivo Stary[2] — [1]Institute of Physics AS CR, Prague, CZ — [2]Institute of Organic Chemistry and Biochemistry AS CR, Prague, CZ

High-resolution AFM images of single molecules brought completely new perspectives in investigation of chemical processes on surfaces. Here we investigated on-surface chemistry of Dibenzo[7]helicene deposited on Ag(111). Annealing above 100C has induced a [4+2] Diels-Alder cycloaddition reaction, which has initiated complex chemical processes on the surface. We have been able to identify an intermediate step and two final products by means of simultaneous AFM/STM measurements with Xe-tip. The intermediate products form complex chiral structures (dimers, trimers and tetramers). To understand the origin of a chiral orientation, we investigated both the racemic mixture and pure (+)-(P) enantiomer of helicene molecules deposited on the Ag(111) surface. We have found that the chiral orientation of the individual molecules as well as their complexes is driven both by chirality of helicene molecules initially deposited on the surface and annealing conditions. We have demonstrated for the first time a chemical control over the final enantiofacial adsorption of non-chiral molecules on the non-chiral metal surface that has resulted in a global mirror-symmetry breaking.

O 5.3 Mon 11:00 S053

Interaction of a Self-assembled Ionic Liquid Adlayer with Graphite(0001) and Reaction with Coadsorbed Lithium — •Florian Buchner[1], Katrin Forster-Tonigold[1], Maral Bozorgchenani[2], Axel Gross[1,3], and R. Jürgen Behm[1,2] — [1]Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, D-89081 Ulm, Germany — [2]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — [3]Ulm University, Institute of Theoretical Chemistry, D-89069 Ulm, Germany

The ionic liquid 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide [BMP][TFSA] is a promising solvent/electrolyte for Li-ion batteries. In this model study we investigated the interaction of (sub-)monolayers of [BMP][TFSA] with a frequently used anode material as graphite(0001) under ultrahigh vacuum (UHV) conditions. Scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and dispersion corrected density functional theory (DFT-D) calculations were employed. After vapor deposition at 300 K and subsequent cool-down to 100 K the STM measurements reveal an ordered (2D) crystalline phase. The row-like adsorption structure is determined by anions and cations which are alternatingly aligned. DFT-D calculations predict that adsorbate-substrate interactions are dispersion interactions, and adsorbate-adsorbate interactions between the ion pairs are equally composed of electrostatic and dispersion interactions. In addition, to mimic an electrolyte, Li was stepwise post-deposited. Subsequent XPS measurements reveal decomposition products of [BMP][TFSA] like LiF, Li_2S, and LiN_3.

O 5.4 Mon 11:15 S053

Direct Observation of Photo-Induced Tautomerization in Single Porphycene Molecules at a Metal Surface — •Hannes Böckmann[1], Shuyi Liu[1], Johannes Mielke[1], Sylvester Gawinkowski[3], Jacek Waluk[3,4], Leonhard Grill[1,2], Martin Wolf[1], and Takashi Kumagai[1] — [1]FHI of the MPG, Berlin, Germany — [2]University of Graz, Graz, Austria — [3]Polish Academy of Sciences, Warsaw, Poland — [4]Cardinal Stefan Wyszyński University, Warsaw, Poland

Molecular switches are of fundamental importance in nature, and photoexcitation is an important stimulus to selectively drive the switching process. However, the local dynamics of these molecules remain far from being completely understood at the single-molecule level. Here we report the direct observation of photo-induced tautomerization in single porphycene molecules on a Cu(111) surface using a combination of LT STM and laser excitation in the near-IR to UV regime. It is found that the thermodynamically stable trans porphycene is converted to the metastable cis form in a unidirectional fashion by photoirradiation. The wavelength dependence of the tautomerization cross section exhibits a steep onset around 2 eV that corresponds to the energy of the d-band edge of the Cu substrate, indicating a surface mediated excitation mechanism. Additionally, a giant isotope effect (about 100) is observed upon substitution with deuterium. Furthermore, we examined the influence of the local environment on the tautomerization by varying the intermolecular interactions via the molecular density and found a decrease in the cross section at high coverage.

O 5.5 Mon 11:30 S053

Vibrationally induced hydrogen-atom transfer in a single porphycene molecule on Cu(110) — •Shuyi Liu[1], Delroy Baugh[1], Xunhua Zhao[1], Sylwester Gawinkowski[2], Jacek Waluk[2], and Takashi Kumagai[1] — [1]Fritz-Haber Institute, Berlin, Germany — [2]Polish Academy of Sciences, Warsaw, Poland

In this talk we present results on the tautomerization of a single porphycene molecules on Cu(110) induced by vibrational excitation via inelastic electron tunneling using an STM. The cis-cis tautomerization was investigated by STS and STM Action Spectroscopy (STM-AS) [1]. STM-AS spectra show steep increases at certain bias voltages, and also exhibits a clear isotope effect when deuterium is substituted for the transferring H-atoms, revealing a vibrationally mediated process. These results indicate excitation of skeletal motion of porphycene plays a crucial role in the reaction. DFT calculations suggest the excited skeletal vibrational mode and N-H(D) stretching transfers energy to the reaction coordinate mode(s) via the anharmonic couplings within the molecule. We also found that the N-H stretching vibration exhibits a noticeable broadening which may be rationalized by strong the anharmonicity of the mode potential that results from the H-bond. Our approach provides a microscopic insight into the electron-vibrational coupling within a single molecule and how it can trigger a chemical reaction. [1] T.K. Prog. Surf. Sci. 90, 239 (2015).

O 5.6 Mon 11:45 S053

Force-induced tautomerization in a single molecule — •Janina N. Ladenthin[1], Thomas Frederiksen[2,3], Mats Persson[4], Sylwester Gawinkowski[5], Jacek Waluk[5], and Takashi Kumagai[1] — [1]Department of Physical Chemistry, Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany. — [2]Donostia International Physics Center, San Sebastián, Spain. — [3]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain. — [4]Surface Science Research Centre and Department of Chemistry, University of Liverpool, UK. — [5]Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland.

Chemical reactions can be activated by heat, electric or light energy. Force is another way but the fundamental process of mechanical activation is much less studied. Force-induced bond breaking and formation are the elementary steps in mechanochemical reactions. However, it remains poorly understood at the single-molecule level. In the talk, we present the force-induced intramolecular H-atom transfer (tautomerization) in a single porphycene molecule on the Cu(110) surface at 5 K using nc-AFM. Porphycene is an intriguing model system for studies of tautomerization [1]. Force spectroscopy was employed to quantify the force needed to trigger the cis-cis tautomerization, revealing a few hundred pN. It was also found that the tautomerization cannot be induced with a Xe-terminated tip, indicating the importance of chemical forces. Furthermore, DFT calculations elucidated the atomistic mechanism behind the force-induced tautomerization.

[1] T. Kumagai et al. PRL 111, 246101 (2013); T. Kumagai et al. Nature Chem. 6, 41 (2014); T. Kumagai, Prog. Surf. Sci. 90, 239 (2015).

O 6: Tribology

Time: Monday 12:00–13:15 Location: S053

Invited Talk O 6.1 Mon 12:00 S053

The surface science of friction: How molecular films affect sliding and plowing — •Roland Bennewitz — INM - Leibniz Institute for New Materials, Saarbrücken, Germany

Two key mechanisms of friction are sliding and plowing. In sliding, adhesive forces between the contacting surfaces lead to friction, in plowing the plastic deformation of the surface. We have studied the role of the molecular structure at the interface in sliding and plowing by friction force microscopy. Results will be presented for plowing friction in a platinum crystal covered by a graphene layer [1]. Adhesive sliding friction can be controlled by macromolecular functionalization of the surfaces [2]. Finally, we will discuss the dynamic shear properties of liquids which exhibit a molecular layering when confined in the sliding contact [3].

[1] Klemenz, A., et al., Atomic Scale Mechanisms of Friction Reduction and Wear Protection by Graphene. Nano Letters, 2014, 14, 7145-7152.

[2] Blass, J., et al., Dynamic effects in friction and adhesion through cooperative rupture and formation of supramolecular bonds. Nanoscale, 2015, 7, 7674-7681.

[3] Krass, M.-D., et al., Dynamic shear force microscopy of nanometer-confined hexadecane layers. J. Phys.: Condens. Matter, 2016.

O 6.2 Mon 12:30 S053

From Static to Sliding Friction: Universal Ageing Law describes Sliding of Metallic Nanoparticles — Michael Feldmann, •Dirk Dietzel, and Andre Schirmeisen — Institute of Applied Physics, Justus Liebig University, Giessen, Germany

Everyday experience teaches us that static and sliding friction are very distinct phenomena: High forces are usually required to initiate sliding, while maintaining a sliding motion causes much less effort. Theoreticians, however, usually link such dynamic friction effects to a common mechanism referred to as contact ageing. While the existence of contact ageing is widely acknowledged (e.g. within rate and state theories) the fundamental processes on the nanoscale are much less clear. Here we will present nanomanipulation experiments of Sb particles on HOPG that will establish a clear correlation between static friction, sliding friction and contact ageing. By analyzing sliding instabilities (i.e. stick slip motion) it is found, that a universal ageing law based on nanorelaxations at the interface is applicable over 6 magnitudes of time and ultimately makes the distinction between static and sliding friction irrelevant.

O 6.3 Mon 12:45 S053

Investingating the transition between stick-slip and smooth sliding with Intermodulation Friction Force Microscopy — •Per-Anders Thorén[1], Astrid de Wijn[2], Riccardo Borgani[1], Daniel Forchheimer[1], and David Haviland[1] — [1]Nanostructure Physics, Royal Institute of Technology, Stockholm, Sweden — [2]Department of Physics, Stockholm University, Stockholm, Sweden

Friction is a complicated phenomenon involving nonlinear dynamics at different scales. The origin of friction is poorly understood, due in part to a lack of methods measuring the force acting on nanometer-scale asperities sliding at velocity of order cm/s. Dispite enormous advances in experimental technique this combination of small length scale and high velocity remained illusive. We present a technique for measuring the velocity-dependence of frictional forces on a single asperity (an AFM tip) reaching velocities up to several cm/s. The method is based on the measurement and analysis of intermodulation products, or frequency mixing of multiple drive tones near a high Q torsional resonance that arise from the nonlinear frictional force. The method gives the oscillation amplitude dependence of both conservative and dissipative dynamic force quadratures, revealing a transition between stick-slip and smooth sliding that is characteristic of friction at high speeds. We can explain the measurements with a modified Prandtl-Tomlinson model that accounts for the viscous and elastic nature of the asperity. With its high force sensitivity for small sliding amplitude, our method enables rapid and detailed surface mapping of the full velocity-dependence of frictional forces to sub 10 nm spatial resolution.

O 6.4 Mon 13:00 S053

Fundamental Surface-Analytical Investigations in Tribology: the Challenges of Studying Phenomena at Sliding Interfaces — •Filippo Mangolini[1], Nitya N. Gosvami[2], J. Brandon McClimon[3], Medard Koshigan[4], James Hilbert[2], Jason A. Bares[2,6], Dalia G. Yablon[5], Julien Fontaine[4], and Robert W. Carpick[2] — [1]School of Mech. Eng., University of Leeds, UK — [2]Dep. of Mech. Eng. and App. Mech., University of Pennsylvania, USA — [3]Dep. of Mat. Sci. and Eng., University of Pennsylvania, USA — [4]LTDS, Ecole Centrale de Lyon, France — [5]SurfaceChar LLC, USA — [6]BorgWarner Powertrain Technical Center, Auburn Hills, USA

Tribology is the study of interacting surfaces in relative motion and the resulting phenomena of friction, lubrication, and wear. The rational design and synthesis of new, modified, and improved materials and lubricants, which can reduce energy and resource consumption in tribological applications, relies on the understanding of the phenomena occurring at sliding interfaces and controlling the observed tribological performance. A key step in the development of this understanding lies in applying advanced surface-analytical methods to the study of tribological materials and interfaces. In this talk, I will present recent experimental results focusing on fundamental surface-analytical investigations of: a) the thermally-induced structural transformations occurring in the near-surface region of a class of solid lubricants, namely amorphous carbon-based materials; and b) the growth of reaction layers formed by antiwear additives used in automotive engine lubricants, gear oils, and greases.

O 7: Graphene I: Structure and Dynamics

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

O 7.1 Mon 10:30 H24

The electronic structure of graphene superlattices revisited — •Pilkwang Kim[1] and Cheol-Hwan Park[2] — [1]Department of Physics and Astronomy, Seoul National University, Seoul, Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul, Korea

We present the calculated electronic structure of graphene superlattices, which are graphenes under lateral, periodic potential. Previous studies on a graphene superlattice [1-3] have reported anisotropic group velocity renormalization, emergence of new zero-energy points, conductance resonance, etc. However, several features manifested in the electronic structure obtained from our numerical calculations, e.g., the movement of the Dirac points in momentum space, cannot be explained by the theories introduced in those studies. In this presentation, we discuss the reason why there are features in the electronic structure of graphene superlattices that were not captured by previous theories. We also discuss electronic structure obtained by using first- and higher-order perturbation calculations.

1.Park, C.-H., Yang, L., Son, Y.-W., Cohen, M. L. & Louie, S. G. New generation of massless Dirac fermions in graphene under external periodic potentials. Phys. Rev. Lett. 101, 126804 (2008). 2.Barbier, M., Vasilopoulos, P. & Peeters, F. M. Dirac electrons in a Kronig-Penney potential: Dispersion relation and transmission periodic in the strength of the barriers. Phys. Rev. B 80, 205415 (2009). 3.Brey, L. & Fertig, H. A. Emerging Zero Modes for Graphene in a Periodic Potential. Phys. Rev. Lett. 103, 046809 (2009).

O 7.2 Mon 10:45 H24

Confinement effects in quasiparticle interference on epitaxial graphene nanoflakes — •Julia Tesch[1], Philipp Leicht[1], Felix Blumenschein[1], Tomas Löfwander[2], Luca Gragnaniello[1], and Mikhail Fonin[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Chalmers University of Technology, Göteborg, Sweden

In the search for suitable materials to be used in nanoscale electronic devices, graphene quantum dots, ribbons and flakes have attracted increased attention amongst researchers, as they allow for a combination of graphene's linear electronic dispersion relation with interesting physical phenomena arising from the size quantization of the structures.

We present a comprehensive study of epitaxial graphene nanoflakes on noble metal surfaces by means of low-temperature scanning tunneling microscopy and spectroscopy. The analysis of quasiparticle interference patterns produced by elastic scattering at defects allows for a clear identification of graphene-related contributions visible as ringlike *inter-* and *intravalley* features within the Fourier transform images [1]. Lateral electronic confinement within these elongated flakes gives rise to additional scattering intensity related to transitions between the flake's transverse modes [2]. Additionally, we discuss the influence of edge configuration, lattice symmetry breaking and quasiparticle lifetime on the scattering, by comparison of the experimental results with tight-binding calculations of realistic graphene nanoflakes.

[1] P. Leicht *et al.*, ACS Nano **8**, 3735 (2014); [2] A. Bergvall *et al.*, Phys. Rev. B **87**, 205431 (2013).

O 7.3 Mon 11:00 H24

Electron interference in ballistic graphene nanoconstrictions — •Johannes Aprojanz[1], Jens Baringhaus[1], Mikkel Settnes[2], Stephen Power[2], Anti-Pekka Jauho[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Technical University of Denmark, DTU Nanotech, Center for Nanostructured Graphene (CNG), 2800 Kgs. Lyngby, Denmark

Graphene nanoconstrictions (GNCs) are a central building block of future carbon electronic devices. However, the synthesis of constrictions with well-defined edges is challenging. Here, we use the tip of a scanning tunneling microscope (STM) for the local etching of graphene, which allows to define GNCs with variable dimensions of down to 1 nm. The GNCs are etched into fully ballistic graphene nanoribbons hosted on the sidewalls of SiC mesa structures [1]. Due to the highly precise etching technique as well as the exceptional electronic quality of the graphene (e.g. mean free path $> 10\ \mu$m), this system is ideal to study coherent transport phenomena. Therefore, the transport characteristics of constrictions with various dimensions are recorded by means of a variable temperature 4-tip-STM. Electron interference at the abrupt graphene interfaces gives rise to characteristic conductance peaks and transport gaps. Their appearance is described by a tight-binding and recursive Green's function approach which especially highlights the robustness of the resonances features against temperature as well as disorder.

[1] Baringhaus et al., Nature **506**, 349 (2014)

O 7.4 Mon 11:15 H24

Graphene on Ru(0001) as a playground for the studies of the graphene-metal interaction — Elena Voloshina[1], Nikolai Berdunov[2], and •Yuriy Dedkov[2,3] — [1]HU Berlin, Germany — [2]SPECS GmbH, Germany — [3]IHP Frankfurt (Oder), Germany

We employ a combination of surface science methods (ARPES, STM/STS, AFM) and DFT calculations for the studies of the lattice mismatched graphene-Ru interface. Our results demonstrate a site-selective interaction (*strong* vs *weak*) between graphene and metal in the moiré lattice. In these studies we show that graphene-*hills* in this structure can be used as an array of electro-mechanical elastic nano-resonantors with very high resonance frequency (in the THz range). On the next step we modify the graphene-Ru interaction via intercalation. Here the scanning probe microscopy and spectroscopy were used to study the crystallographic structure and electronic properties of the uniform free-standing graphene layers obtained by intercalation of oxygen monolayer in the *strongly* bonded graphene/Ru(0001) interface. Spectroscopic data show that such graphene layer is heavily *p*-doped with the Dirac point located at 552 meV above the Fermi level, that corroborates our ARPES data. Experimental data are understood within DFT and the observed effects are in good agreement with the theoretical data.

Invited Talk O 7.5 Mon 11:30 H24

Direct view on non-equilibrium carriers in graphene with time-resolved ARPES — •Isabella Gierz — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The linear band structure of graphene bares great potential for optoelectronic applications ranging from Terahertz lasing to efficient light harvesting. We explore the response of the Dirac carriers in lightly hole-doped epitaxial graphene samples to three different excitation schemes: interband transitions for $\hbar\omega_{\mathrm{pump}} > 2\mu_{\mathrm{e}}$, free carrier absorption for $\hbar\omega_{\mathrm{pump}} < 2\mu_{\mathrm{e}}$, and resonant phonon excitation for $\hbar\omega_{\mathrm{pump}} = 200\,\mathrm{meV}$. Time- and angle-resolved photoemission spectroscopy (tr-ARPES) allows us to map the transient population of the Dirac cone in momentum space over a large energy window of several electron Volts down to arbitrarily small excitation energies.

We find a short-lived population-inverted state for interband excitation [1], a simple metallic relaxation behaviour for free carrier absorption [1], and indications for a transient enhancement of the electron-phonon coupling constant when resonantly driving the in-plane phonon in bilayer graphene [2]. Furthermore, by improving the temporal resolution to $\sim$10 fs, we were able to identify impact ionization as the primary thermalization channel within the first $\sim$25 fs [3].

[1] Gierz et al., Nature Materials 12, 1119 (2013)
[2] Gierz et al., PRL 114, 125503 (2015)
[3] Gierz et al., PRL 115, 086803 (2015)

O 7.6 Mon 12:00 H24

Electronic properties of ytterbium interaction with graphene on Ir(111) — Hendrik Vita[1], •Stefan Böttcher[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany

The intercalation of metals in between graphene monolayers and a substrate is interesting from several points of view, for example in order to understand the effect of symmetry lowering in the interaction of the metal states with the specific graphene π bands in the region of the "Dirac cone". Here we present a study of the intercalation of a rare earth metal, Yb, in between graphene and Ir(111). Ytterbium exhibits an s-type valence band, making it possible to compare the electronic structure to the widely studied cases of alkali metals used as intercalates in graphene intercalation compounds. Using core level spectroscopy we follow the deposition of Yb and the evolution of the intercalated phase. LEED studies show that the structural arrangement of the intercalated Yb thin film leads to a $(\sqrt{3}\times\sqrt{3})$R30° phase. Angle-resolved photoemission reveals that the interaction between the metal states and the graphene π band near the K point induces an extremely strong n-type doping. Hybridization-induced band gaps open in the π band at binding energies of 0.3 eV and 1.6 eV due to the interaction with the strongly localized metal $4f$ states. We compare our data with other weakly and strongly interacting intercalated metal layers.

O 7.7 Mon 12:15 H24

Plasma-assisted CVD graphene synthesis and characterization on nickel substrates — •Patricia Pop-Ghe, Lisa Krückemeier, Nicolas Wöhrl, and Volker Buck — Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr, 1, 47057 Duisburg, Germany

This work presents the synthesis of graphene by plasma-assisted chemical vapour deposition on polycrystalline nickel foils. It is initiated by the comparison of the mechanisms in CVD and plasma-assisted CVD on a nickel substrate and focusses on the development of a growth model for both sides of the substrate within the experimental results. In detail, the differences in graphene growth at the front and at the back side of the substrate are investigated and correlated to specific influence factors. It is shown that growth mode as well as expansion and quality of graphene sheets can be adjusted by process temperature and time respectively since carbon solubility and diffusion in nickel both hold strong temperature and time dependencies. The strong time dependance of graphene growth is further indicative of a reconstructional nature of graphene formation, which is further discussed in the developed growth model. In addition the influence of the substrate is investigated by comparing results from graphene growth on polycrystalline nickel foils and nickel single crystal(111) substrates, as well as graphene on nickel (synthesized graphene) and silicon dioxide substrates (transferred graphene). Raman mappings are demonstrated to confirm the quality of the synthesized graphene.

O 7.8 Mon 12:30 H24

Determination of the optical constants of graphene at the carbon K-edge by transmission spectroscopy — •Christine Jansing[1], Hans-Christoph Mertins[1], Andreas Gaupp[1], Andrey Sokolov[2], Markus Gilbert[1], Andreas Schümmer[1], Hud Wahab[3], Heiko Timmers[3], Suk-Ho Choi[4], and Dominik Legut[5] — [1]Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — [2]HZB, Albert Einstein Str. 15, D-12489 Berlin — [3]University of New South Wales, Canberra, ACT 2600, Australia — [4]Kyung Hee University, Yongin 446-701, Korea — [5]IT4Innovations Center, VSB-Technical University of Ostrava, CZ-708 33 Ostrava, Czech Republic

The transmission of linearly polarized synchrotron radiation through quasi-free-standing graphene, supported by a Si3N4-membrane, has been measured across the carbon K-edge. From the measured absorption spectrum, that represents the imaginary part, the real part of the refractive index has been extracted via a Kramers-Kronig transformation. Based on these detailed optical parameters, reflection spectra have been simulated for linearly polarized soft x-ray light incident on graphene-metal systems. Importantly, the simulations include the interference of light reflected from graphene and from light reflected from the metallic substrate, respectively. In addition the optical constants are compared to the ones obtained by various density function theory calculations using single-electron framework as well as the more complex many-body approaches to the electronic structure of free-standing graphene.

O 7.9 Mon 12:45 H24

Origins of contact resistance in graphene-metal edge-contacts — •Bernhard Kretz[1], Christian Søndergaard Pedersen[2], Daniele Stradi[2], Aran Garcia-Lekue[1,3], and Mads Brandbyge[2] — [1]Donostia International Physics Center, E-20018 San Sebastian, Spain — [2]Center for Nanostructured Graphene, DTU Nanotech, Tech. Uni. of Denmark, DK-2800 Kongens Lyngby, Denmark — [3]IKERBASQUE, Basque Foundation for Science, E-48013 Bilbao, Spain

The transport properties of graphene-metal contacts play an important role in the design of graphene-based devices. Recent studies demonstrate the advantages of the edge-contact geometry over conventional surface contacts.[1,2] However, significantly different conclusions are reached regarding the influence of the metal on the conductance properties of edge-contacts: while simulations indicate that the contact resistance is of the same order of magnitude for different metals,[2] experiments reveal a strong metal-dependence.[1] The possible origins of these discrepancies are explored by studying the transport properties of graphene edge-contacts with different metals, different edge conformations, terminations and adsorption distances. We employ a density functional theory (DFT) based non-equilibrium Green-function (NEGF) approach, using the TranSIESTA code. Our results will offer insights towards a better understanding of the conductance properties of graphene-metal contacts deviating from ideal interfaces.

[1] Wang et al. Science 342, 2013; Chu et al. ACS Nano 8, 2014

[2] Matsuda et al., J. Phys. Chem. C 114, 2010

O 7.10 Mon 13:00 H24

Magnetically confined quantum dots in graphene revealed by scanning tunneling spectroscopy — •Nils Freitag[1], Peter Nemes-Incze[1], Larisa Chizova[2], Colin R. Woods[3], Roman V. Gorbachev[3], Yang Cao[3], Andre K. Geim[3], Kostya S. Novoselov[3], Florian Libisch[2], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen, Otto-Blumenthal Street, 52074 Aachen, Germany — [2]Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria — [3]School of Physics & Astronomy, University of Manchester, Manchester, United Kingdom

Confining graphene's chiral massless charge carriers by carving out nano-structures to circumvent Klein-tunneling suffers from disordered edges, impeding the control of the quasi-relativistic particles. Here, we use the electrostatic potential of an STM tip in combination with an homogeneous magnetic field to confine electrons in graphene without edges[1]. The confinement becomes visible as a fourfold charging sequence at B>2T, as expected from valley and spin degeneracy. Up to 40 charging peaks are observed in the hole and electron sector with charging energies of 5-10meV. Characteristic spatial charging patterns created by potential modulations of the commensurate G on BN are found[2].

[1] G. Giavaras and F. Nori, PRB 85, 165446 (2012)

[2] C. R. Woods et al., Nat. Phys. 10(6), 451-456 (2014)

O 7.11 Mon 13:15 H24

Controling intramolecular Hydrogen-transfer by Gate-tunable STM — •Shai Mangel[1], Christian Dette[1], Katharina Polyudov[1], Paul Punke[1], Roberto Urcuyo[1], Marko Burghard[1], Soon Jung Jung[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, D-70569 Stuttgart — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The atomic level control of the electron transport has important advantages for many applications, such as molecular electronics, solar cells and sensors. Electron transport properties can be controlled by the intramolecular reaction which reshape the electronic configuration without any significant change in the conformation. The STM-induced tautomerization, i.e the interconversion between two isomers due to the migration of Hydrogen, was observed in the form of telegraphic noise. Several methods to control the intramolecular Hydrogen-transfer by changing the chemical environment of the molecule have been developed, such as locating adatoms or introducing defects. However, these affect the molecules only in the nm range. In this work, using the gate-tunable STM, we demonstrate a global control of the chemical environment of the substrate which results in the changing of the switching rate of the Hydrogen-transfer. The system we have used is a molecular network of phthalocyanine on graphene. Understanding and controlling the influence of the field-effect on the molecules, will be crucial for the construction of future molecular devices for energy and information usages.

O 8: Surface State Spectroscopy I

Time: Monday 10:30–13:00 Location: H4

O 8.1 Mon 10:30 H4

One-step theory of two-photon photoemission — •Jürgen Braun[1], Roman Rausch[2], Michael Potthoff[2], Jan Minar[1], and Hubert Ebert[1] — [1]LMU München — [2]Universität Hamburg

A general theoretical framework for the description of pump-probe photoemission is presented. The approach is based on a general formulation using the Keldysh formalism for the lesser Green function to describe the real-time evolution of the electronic degrees of freedom in the initial state after a strong pump pulse that drives the system out of equilibrium. The final state is represented by a time-reversed low-energy electron diffraction (LEED) state. The formalism allows for a quantitative calculation of the time-dependent photocurrent that results from core or valence-band excitations, and is applicable to simple metals or more complex materials like topological insulators. Our approach covers as a special case the two-photon photoemission (2PPE) scenario where both the pump-pulse and the probe pulse are weak in intensity. We present as a first application of our fully relativistic implementation within the Munich SPR-KKR package [2] calculated 2PPE spectra from Ag(100), where the first image state serves as intermediate state to probe the occupied bandstructure below the Fermi level [3].

1. J. Braun, R. Rausch, M. Potthoff, J. Minar, H. Ebert, Phys. Rev. B 91, 035119 (2014)
2. H. Ebert et al., The Munich SPR-KKR package, version 6.3, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2012)
3. J. Braun, R. Rausch, M. Potthoff, J. Minar, H. Ebert, submitted

O 8.2 Mon 10:45 H4

Tempereture dependent one-step model of ARPES: effects of spinfluctuations and phonons — •Jan Minar[1,2], Sergey Mankovsky[1], Jurgen Braun[1], and Hubert Ebert[1] — [1]LMU München, Germany — [2]University of West Bohemia, Plzen, Czech Rep.

Various technical developments widened the potential of angle-resolved photo-emission (ARPES) tremendously during the last one or two decades. In particular improved momentum, energy and spin resolution as well as the use of photon energies from few eV up to several keV makes ARPES a rather unique tool to investigate the electronic properties of solids and surfaces. Here, we present a generalization of the state of the art description of the photoemisison process, the so called one-step model that describes excitation, transport to the surface and escape into the vacuum in a coherent way. In particular, we present an theoretical description of the temperature dependent ARPES with the emphasis on spin fluctuations. Effects of finite temperatures are included by the so called alloy analogy model (based on the coherent potential approximation) which allows to describe uncorelated lattice vibrations in combination with spin fluctuations on the same footing.

Invited Talk O 8.3 Mon 11:00 H4

Momentum Microscopy with Time-of-Flight Analysis and Spin Filtering: Direct Imaging of k-Space Objects and Spin Textures — •Gerd Schönhense — Institut für Physik, Johannes Gutenberg-Universität, 55128 Mainz, Germany

Momentum microscopy has recently set impressive benchmarks, in particular in combination with an imaging spin filter [1]. In Mainz we develop a modified approach based on time-of-flight parallel energy detection instead of dispersive analyzers [2]. A fast delay-line detector ($>$ 5 Mcps, 150 ps resolution) provides 3D data recording. The state of development and first scientific results will be reported. The spin-filtered mode was explored at BESSY II (U125-2 NIM) for determination of P(E_B,k_x,k_y) spin textures with more than 10^4 data points simultaneously. Surface and bulk bands of the topological ferroelectric GeTe(111) show Rashba-type spin textures [3]. For W(110) three surface bands with anomalous spin textures were found [4], one of which has been studied before [5]. In the soft-X range (PETRA III, P04) we observed sharp 3D band patterns with giant CDAD asymmetries for Ir and W up to hν=1300eV at T=30K, with 10^5-10^6 data voxels simultaneously. Variation of photon energy yielded I(E_B,k_x,k_y, k_z) datasets for Fermi surface tomography. Strategies to utilize multibunch modes are explored at MAXLAB (Lund, Sweden).

[1] Tusche et al., Ultramicroscopy DOI: 10.1016/j.ultramic.2015.03.020 (2015); [2] Schoenhense et al., JESRP 200 (2015) 94 ; [3] Elmers et al., this conf.; [4] Kutnyakhov et al., this conf.; [5] Miyamoto et al., PRL 108 (2012) 066808.

O 8.4 Mon 11:30 H4

Fast Band-Mapping in the Soft X-Ray Range Using ToF Momentum Microscopy — •K. Medjanik[1,2], O. Fedchenko[1], S. Chernov[1], D. Kutnyakhov[1], B. Schönhense[3], M. Ellguth[1], A. Oelsner[4], S. Däster[5], Y. Acremann[5], T. Peixoto[6], P. Lutz[6], C.-H. Min[6], F. Reinert[6], J. Viefhaus[7], W. Wurth[8,9], H.J. Elmers[1], and G. Schönhense[1] — [1]Institut für Physik, Uni-Mainz — [2]MAX IV Lab., Lund, Sweden — [3]Imperial College, London, UK — [4]Surface Concept GmbH — [5]ETH Zürich — [6]EP 7, Uni-Wuerzburg — [7]DESY, Hamburg — [8]CFEL, Uni-Hamburg — [9]Desy Photon Science

We present the first results of time-of-flight k-microscopy [1] using soft X-rays. The full 3D Brillouin zones of W and Ir were mapped at beamline P04 of PETRA III between hv=300 and 1300eV. Parallel acquisition of k-discs with 18,000 data points each and about 100 energies resulted in orders of magnitude higher speed and allowed us to operate the monochromator down to its resolution limit of 40,000 at 1000eV. The band features are sharp up to 1300eV at T=30K. Transfer of photon momentum manifests in the form of a rigid shift of the k_x,k_y-patterns and corresponding energy shift. The 40-bunch mode of PETRA provides an ideal pulse period of 192 ns. In order to adapt the ToF-microscope to multibunch conditions or to pump-probe conditions with low-repetitive lasers, a fast electrostatic chopper is developed [2].

Funded by BMBF (05K13UM2, 05K13GU3)

[1] G.Schönhense et al., JESRP 200 (2015) 94-118; [2] A. Zaporozhchenko et al., DPG 2016.

O 8.5 Mon 11:45 H4

The Adsorption Structure of Cobalt Tetraphenylporphyrin on Ag(100) — •Daniel Wechsler, Quratulain Tariq, Matthias Franke, Liang Zhang, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany

Knowledge about the adsorption structure of large organic molecules on single-crystal surfaces is crucial to control how molecules self-assemble on surfaces. We have studied the adsorption structure of cobalt(II) 5,10,15,20-tetraphenylporphyrin (CoTPP) deposited on Ag(100) with low energy electron diffraction (LEED), synchrotron-radiation photoelectron spectroscopy (SRPES), X-ray standing wave (XSW) and near edge X-ray absorption fine structure (NEXAFS). Differences in the LEED patterns show a coverage-dependent unit cell change. From SRPES, XSW and NEXAFS, we were able to determine the atomic height with respect to the surface, the rotational angle of the phenyl rings, and the distortion of the macrocycle. The project is supported by the DFG through FOR 1878 (funCOS).

O 8.6 Mon 12:00 H4

Ab initio core-level spectroscopy for large systems: Comparison of ground-state density-functional based approximations — •Georg S. Michelitsch, Katharina Diller, Reinhard J. Maurer, and Karsten Reuter — Technische Universität München

Core-level spectroscopy experiments such as Near-Edge X-Ray Absorption Fine-Structure (NEXAFS) allow to sensitively probe the electronic states of gas-phase and surface-adsorbate systems. Particularly for surface-adsorbate systems the complexity of the experimental signatures requires independent first-principles calculations for a reliable analysis. For corresponding system sizes, numerically efficient core-level constraining approaches based on density-functional theory (DFT) are presently the method of choice. Different flavors of this approximate approach vary by different occupations of both the initial core level and the final virtual orbital participating in the electron excitation processes. We systematically benchmark these flavors against experimental K-edge data from a library of organic compounds representing building blocks of organic adsorbates like benzene or porphine. Assessing different DFT functionals, we generally find relative peak positions in the near-edge region to already be well reproduced at the semi-local level. With respect to the different flavors the transition potential approach [1] consistently yields most reliable transition energies and intensities.

[1] L. Triguero, L.G.M. Petterson, and H. Agren, Phys. Rev. B 58,

8097 (1998).

O 8.7 Mon 12:15 H4

Edge states at vacancy islands on pristine Ni(111) — •Martin Schmitt[1], Jeannette Kemmer[1], Matthias Vogt[1], Matthias Bode[1], Mara Gutzeit[2], Paolo Ferriani[2], and Stefan Heinze[2] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts Universität zu Kiel, Leibnizstr. 15, 24098 Kiel, Germany

Recently, the dispersion relations of surface electronic states of pristine Ni(111) has been probed by quasiparticle interference (QPI) [1]. In agreement with earlier inverse photoemission experiments [2] an exchange-split and upward dispersing Shockley-type *sp*-derived surface state was observed. In a follow-up investigation we have studied the electronic properties of step edges surrounding hexagonally shaped vacancy islands by means of low-temperature scanning tunneling spectroscopy. Our results indicate that *A*- or *B*-steps are markedly different. While one type of step edge is essentially featureless, local tunneling spectra measured on the other exhibit an additional peak. By comparison with density functional theory calculations we discuss if this peak can potentially be interpreted as a one-dimensional edge state.

[1] A. Krönlein *et al.*, Phys. Rev. B **89**, 155413 (2014).
[2] M. Donath *et al.*, Phys. Rev. Lett. **70**, 2802 (1993).

O 8.8 Mon 12:30 H4

Polaron driven structural reconstruction in Rutile TiO_2(110) — •Michele Reticcioli[1], Xianfeng Hao[2], Martin Setvin[3], Ulrike Diebold[3], and Cesare Franchini[1] — [1]University of Vienna — [2]Yanshan University — [3]Vienna University of Technology

The role of polarons in TiO_2 is of key importance for understanding the fundamental properties and functionalities of this material. In this work we use density functional theory with an on-site Coulomb interaction U and molecular dynamics to study the formation and dynamics of small polarons in the reduced rutile TiO_2(110) surface. Our theoretical results are validated by a direct comparison with STM data. We show that excess electrons donated by oxygen vacancies (V_O) form small polarons preferentially in subsurface Ti sites, and that polarons easily hop to neighboring sites in the subsurface and surface layers. The polaron stability (in terms of the polaron formation energy) has been examined as a function of V_O concentration (5.5%, 11%, 16.6% and 22.2%) by adopting a large (9×2) supercell. It is found that polaron formation become more favorable by increasing V_O concentration due to the lower energy cost to distort the lattice, which is needed to provide the lattice with the necessary flexibility to host self-trapped electrons. At high polaron concentration the polaron-polaron repulsion weakens this trend and drives the system towards an instability, falling into a reconstruction of the surface. The polaron driven surface reconstruction has been studied for two particular suggested structures, named Ti_2O_3-(1×2) and Ti_2O-(1×2). Hence the convenience of the reconstruction with respect to the thermodynamic conditions has been clarified.

O 8.9 Mon 12:45 H4

Evidence for an extremely low-lying electron-hole excitation mode in the Sb(111)-phonon dispersion measured by HAS — •Patrick Kraus[1], Florian Apolloner[1], Christian Gösweiner[1], Giorgio Benedek[2,3], and Wolfgang E. Ernst[1] — [1]Institute of Experimental Physics, Graz Univerity of Technology, Graz, Austria — [2]Donostia International Physics Center (DIPC), San Sebastian/Donostia, Spain — [3]Dipartimiento di Scienza dei Materiali, Universita di Milano-Bicocca, Milano, Italy

The semimetal antimony (Sb) is an attractive candidate for studying the properties of topological surfaces. Quite recently the surface phonon dispersion curve of Sb(111) as well as the influences of electron-phonon interactions were calculated using DFPT. However, there has been a shortage of experimental data for comparison and verification of the models used. Hence, measurements on antimony are long overdue. As a surface sensitive technique, Helium Atom Scattering (HAS) allows investigating elastic as well as inelastic phenomena associated with structure and dynamics of the electronic corrugation slightly above the Sb(111) surface. Besides confirming the expected surface phonon dispersion curves, recent inelastic HAS measurements on Sb(111) revealed multiple unexpected branches. One of them, lying completely below the Rayleigh curve of the phonon dispersion with a maximum energy at the K-point below 3*meV, can not be assigned to any known feature up to now. The electronic peculiarities in the case of Sb(111) can lead to the formation of defined electon-hole excitation branches which may be detected via iHAS measurements.

O 9: Nanostructures at Surfaces I

Time: Monday 10:30–12:45 Location: H6

O 9.1 Mon 10:30 H6

Fabrication of nanostructures on thin organic layers by Focused Electron Beam Induced Processing — •Martin Drost[1], Fan Tu[1], Florian Vollnhals[1], Imre Szenti[2], Janos Kiss[2], Hans-Peter Steinrück[1], and Hubertus Marbach[1] — [1]Physik. Chemie II, FAU Erlangen-Nürnberg, GER — [2]MTA-SZTE Reaction Kin. and Surf. Chem. Research Group, Un. of Szeged, HUN

Focused Electron Beam Induced Processing (FEBIP) comprises several nanofabrication techniques in which a focused electron beam of an electron microscope is used to modify the properties of adsorbed precursor molecules or the substrate itself. We demonstrate that it is possible to fabricate nanostructures using FEBIP with the precursors Co(CO)3NO and Fe(CO)5, on Si(111) and TiO2(110), both precovered with several layers of 2H-Tetraphenylporphyrin (2HTPP). At room temperature, both pristine surfaces are catalytically active towards the decomposition of Co(CO)3NO, leading to growth of a granular film, whereas EBID with Fe(CO)5 is selective. The catalytic activity of the pristine surfaces towards decomposition of Co(CO)3NO can be inhibited by a thin 2HTPP layer. On the corresponding organic interfaces it is possible to selectively fabricate nanostructures using FEBIP, with both precursors. The deposits are characterized by Scanning Electron Microscopy (SEM) and local Auger Electron Spectroscopy (AES). Supported by the DFG through grant MA 4246/1-2, research unit FOR 1878/funCOS; COST Action CM1301; Excellence Cluster EAM of the FAU Erlangen-Nürnberg.

O 9.2 Mon 10:45 H6

Nanostructures fabricated via Focused X-ray Beam Induced Deposition (FXBID) — •Fan Tu, Martin Drost, Florian Vollnhals, Andreas Späth, Krick Calderon Sandra, Rainer H. Fink, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr.3, D-91058, Erlangen, Germany

We will report the usage of a focused monochromatic X-ray beam for the fabrication of nanostructures by the local dissociation of adsorbed precursor molecules. A particular appealing aspect of monochromatic X-rays is thereby the potential to selectively address certain atoms and/or bonds within the precursor molecule and thus tuning the decomposition process. It has been proposed that especially the Auger decay process following the creation of a core hole by photoabsorption causes the selective dissociation of different bonds [1]. The local X-ray irradiation and the successive characterization were conducted at the PolLux beamline at the Swiss light source with a scanning transmission X-ray microscope (STXM). X-ray energy dependent deposition of Cobalt and Manganese carbonyl precursors will be investigated. The Chemical composition and the deposition yield were characterized by in-situ X-ray adsorption spectroscopy (XAS) in the STXM instrument.

Supported by the DFG via grant MA 4246/1-2, MA 4246/2-1, the cluster of excellence Engineering of Advanced Materials at the FAU Erlangen-Nürnberg and two granted beamtimes at the PolLux STXM of Swiss Light Source.

[1] Cazaux, J. Microsc. 188(1997), 106

O 9.3 Mon 11:00 H6

Vertically aligned MWCNTs on glassy carbon: A nanostructured all carbon electrode — •Eser Metin Akinoglu[1,2], Ömer Akay[1], and Michael Giersig[1,3] — [1]Freie Universität Berlin , Department of Physics, 14195 Berlin, Germany — [2]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam-Golm Science Park, 14476 Potsdam, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut Nanoarchitekturen für die Energieumwandlung, 14109 Berlin, Germany

Multi-walled carbon nanotubes (MWCNTs) are known for their unique mechanical and electronic properties and find applications in many aspects of science. MWCNTs as a powder have been shown to be extraordinary supports for catalytically active materials where they are beneficial for surface area enhancement effects as well as for charge separation and transport. Another carbon material, namely glassy carbon, is widely used in electrochemistry as an electrode material due to its high conductivity, high corrosion resistance and abundance of carbon. In this contribution we present a nanostructured all carbon electrode that is based on vertically aligned MWCNTs directly grown on glassy carbon via plasma enhanced chemical vapor deposition. Besides structural and electronic characterization of our materials we show first applications of our concept towards highly conductive, inexpencive nanostructured high surface area electrodes.

O 9.4 Mon 11:15 H6

Correlation of scanning x-ray microscopy and HRTEM measurements of carbon nanomaterials — •Fabian Fritz[1,2], Rasmus Westerström[3], Lothar Houben[4], Martina Luysberg[4], Alexey A. Popov[5], Claus M. Schneider[2], and Carola Meyer[1] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, Germany — [3]Physik-Institut, Universität Zürich, Switzerland — [4]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich GmbH, Germany — [5]Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany

High resolution transmission electron microscopy (HRTEM) is often used to study the structure of nanomaterials. Scanning transmission x-ray microscopy (STXM) is a synchrotron based nano-spectroscopy technique for recording nano-scaled images with chemical and magnetic contrast.

Here we present a combined HRTEM and STXM study of carbon nanotube (CNT) bundles filled with $Er_3N@C_{80}$ fullerenes. The measurements demonstrate that unique CNT bundles can be located and studied with the two techniques. We also obtained erbium M5 edge x-ray absorption spectra from a single bundle. Images recorded on and off resonance provide an erbium map of the sample.

We correlate HRTEM and STXM images of the same nanometer scaled object and discuss the combination of the two techniques.

O 9.5 Mon 11:30 H6

Covalent or organometallic networks? A comparative study of a dibromo-diiodo-pyrene derivate on Ag(111) vs. Au (111) by XPS, NEXAFS, and STM — •Matthias Lischka[1,2], Johanna Eichhorn[1,2], Massimo Fritton[1,2], Thomas Strunskus[3], Vijay Vyas[4], Wolfgang M. Heckl[1,2,5], and Markus Lackinger[1,2,5] — [1]Department of Physics, TU München, James-Franck-Str. 1, 85748 Garching — [2]Center for NanoScience, Schellingstr. 4, 80799 Munich — [3]Institute for Materials Science - Multicomponent Materials, Christian-Albrechts- Universität zu Kiel, Kaiserstr. 2, 24143 Kiel — [4]MPI für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart — [5]Deutsches Museum, Museumsinsel 1, 80538 Munich

The thermally activated surface chemistry of a dibromo-diiodo-pyrene is comparatively studied on Ag(111) and Au (111) under ultrahigh vacuum conditions. X-ray photoelectron spectroscopy of C 1s, Br 3d, and I 3d was used to identify chemical changes that indicated the occurrence of two distinct phases for both surfaces. Upon progressive heating on Ag (111), an initially formed partly organometallic phase becomes fully organometallic. On Au (111) at room temperature, however the precursor is already deionated and partially forms covalent bonds. Further heating drives debromination and results in conversion to a fully covalent network. The structural characterization of each phase is carried out by a combination of high resolution scanning tunneling microscopy and C 1s near edge x-ray absorption fine structure. Special emphasis is put on buckling in the networks as a consequence of covalent bond formation due to steric hindrance.

O 9.6 Mon 11:45 H6

Probing reactive metal atoms on functionalized surfaces by porphyrin metalation — •Jan Nowakowski[1], Sylwia Nowakowska[2], Gitika Srivastava[1], Milos Baljozovic[1], Jan Girovsky[1], Nirmalya Ballav[3], and Thomas A. Jung[1] — [1]Paul Scherrer Institute, Villigen, Switzerland — [2]University of Basel, Switzerland — [3]IISER Pune, India

On-surface metalation of porphyrins has been established on a wide range of surfaces including atomically clean metallic substrates [1] as well as metal-oxides [2] and metallic surfaces modified by oxygen [3]. In this contribution [4], we use the well-studied metalation reaction to present evidence that Cl- and N-induced modifications of the top-most surface layer (i.e. adsorbate-induced surface superstructures) on Cu(001) have decisive and contrasting impact on the reactivity of the surface, as well as on molecular self-assembly. The N superstructure facilitates the metalation reaction and self-assembled domains of CuTPP are formed at room temperature. On the contrary, the Cl superstructure fully inhibits the reaction and causes 2HTPP to assemble into small 'magic' clusters. A spectro-microscopy correlation approach combining X-ray Photoelectron Spectroscopy, Ultraviolet Photoelectron Spectroscopy, Low Energy Electron Diffraction and Scanning Tunnelling Microscopy has been used in this study.

[1] Auwärter, W. et al., ChemPhysChem 8, 250 (2007); [2] Wang, C. et al., Chem Commun 50, 8291 (2014); [3] Nowakowski J. et al., Chem. Commun., 49, 2347 (2013); [4] Nowakowski J. et al., submitted.

O 9.7 Mon 12:00 H6

Controlled creation and imaging of quantum states of dangling bond structures on H-terminated Si(001) — •Asif M Suleman, Kian A Rahnejat, Cyrus F Hirjibehedin, Neil J Curson, Gabriel Aeppli, David R Bowler, and Steven R Schofield — University College London, London, UK

An understanding of how semiconductor point defects interact is needed if they are to fulfil their potential as the basis of future nanoelectronic and quantum devices. Scanning tunnelling microscopy (STM) has been used to investigate point defects on semiconductor surfaces. Here we present an investigation of interacting dangling bond (DB) orbitals on H-terminated Si(001). The STM tip is used to selectively desorb individual H atoms to create a DB [1]. Pairs, or dimers, of DBs interact as their individual excited states overlap, signalled by the appearance of a bright protrusion between them in a molecular-like state [2]. Tip-induced band bending calculations show this excited molecular state of the dimer come into tunnelling range at high biases and low currents. The energy alignment with the tip Fermi level is also affected by additional DBs in the vicinity of the dimer. 2D structures of DBs, including trimers and tetramers, were produced that exhibit 2D extended excited molecular states that we present here for the first time. By modelling each DB with a 2D Pöschl-Teller potential well holding two bound states, we could simulate the bound states for the DB structure and find good agreement with experiment. [1] J. W. Lyding *et al. Appl. Phys. Lett.* **64**, 2010 (1994). [2] S. R. Schofield *et al. Nat. Commun.* **4**, 1649 (2013). [3] A. M. Suleman *et al. In prep.* (2015).

O 9.8 Mon 12:15 H6

Interaction of dangling bond bound states on boron passivated Si(111) — •Manuel Siegl — London Centre for Nanotechnology University College London 17-19 Gordon St London WC1H 0AH United Kingdom

Scanning tunnelling microscopy (STM) was used in the creation of quantum structures such as quantum corrals showing bound electron states across multiple lattice sites on a Fermi-level pinned metal surface [1]. Taking degenerately boron doped Si(111), we extend STM-imaging to spatially resolved scanning tunnelling spectroscopy maps (CITS) [2] in order to examine the electronic structure of point defect induced bound states on a semiconductor Fermi-level pinned surface [3]. We investigate the site dependent interaction of these atomic size quantum dots in varying arrangements, with changing dangling bond separation and crystallographic direction. The experimental results are then compared to first principle density function theory (DFT) calculations and we confirm a non-linear constructive interference between the excited states of positively charged dangling bonds [4].

References [1] M. F. Crommie et al., Science 262, 218 (1998). [2] R. J. Hamers et al., PRL 56, 18 (1986). [3] M. Berthe et al., PRL 97, 206801 (2006) [4] H. Hedgeland, M. Siegl et al. In preparation (2016).

O 9.9 Mon 12:30 H6

Morphology and Environment dependent Luminescence of Dye Aggregates — •Mohammadreza Bahrami[1], Sven Kraft[1], Tamam Bohamud[1], Kai Wardelmann[1], Björn Vogler[1], Johannes A.A.W. Elemans[2], Ingo Barke[1], and Sylvia Speller[1] — [1]University of Rostock, Institute of Physics, 18059 Rostock, Germany — [2]Radboud University Nijmegen, Institute for Molecules and

Materials, 6525 AJ Nijmegen, The Netherlands

We study the spatially resolved photoluminescence, as one of the relaxation pathways of excitons, from Copper-based porphyrin [1] aggregates which form on surfaces via self-organization. Among the different observed morphological motifs of the aggregates we focus on isotropic aggregates as well as branched strands with typical heights between 30 and 150 nm. Fluorescence and phosphorescence microscopy images show different intensity from these two morphologies. Utilizing atomic force microscopy we correlate photoluminescence and structural properties to elaborate on possible reasons of such morphology-dependent luminescence. We further present our results on the effect of metallic nanostructures in the vicinity of the aggregates and address the role of these metal systems as local sources of enhanced excitation fields.

[1] M.J.J. Coenen, et al., Phys. Chem. Chem. Phys. **15**, 12451 (2013)

O 10: Two-dimensional Materials

Time: Monday 9:30–13:00 Location: H16

O 10.1 Mon 9:30 H16

Boundary conditions for transition-metal dichalcogenide monolayers in the continuum model — •Csaba Géza Péterfalvi, Andor Kormányos, and Guido Burkard — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

We derive the boundary conditions for MoS$_2$ and similar transition-metal dichalcogenide honeycomb (2H polytype) monolayers with the same type of $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian within the continuum model around the K points. [1] In an effective 2-band description, the electron-hole symmetry breaking quadratic terms are also taken into account. We model the effect of the edges with a linear edge constraint method that has been applied previously to graphene. Focusing mainly on zigzag edges, we find that different reconstruction geometries with different edge-atoms can generally be described with one scalar parameter varying between 0 and 2π. We analyze the edge states and their dispersion relation in MoS$_2$ in particular, and we find good agreement with the results of previous density functional theory calculations for various edge types.

[1] Cs. G. Péterfalvi, A. Kormányos, G. Burkard, arXiv:1509.00184 (2015).

O 10.2 Mon 9:45 H16

High Q-factor in WSe2 Nano-electromechanical resonator — •Antoine Reserbat-Plantey[1], Nicolas Morell[1], Ioannis Tsioutsios[1], Kevin Schädler[1], François Dubin[2], Frank Koppens[1], and Adrian Bachtold[1] — [1]ICFO, The Insitutue for Photonic Sciences, Barcelona, ES — [2]INSP, Université Paris 6, Paris, FR

Atomically thin nano-electromechanical systems (2D-NEMS) combine extremely low mass resonators having resonant frequencies in the MHz-GHz range, wide tunability, low damping and exotic non-linearities. Atomically thin 2D semi-conductors such as transition metal dichalcogenides (TMD) have extremely rich optical properties (direct band gap, spin valley, embedded quantum emitters), which are intrinsically linked to their low dimensionality. Optical and electronic properties of WSe2, an emblematic TMD, have been intensively studied while there is no extensive nanomechanical investigation of this system. Here we show a new generation of semiconductor 2D-NEMS made of monolayer of WSe2. We record mechanical and photoluminescence spectra of WSe2 nanoresonators down to cryogenic temperatures. We measure mechanical quality factor $Q>47000$ at $T=3.5$ K, which is the highest value reported so far for 2D-NEMS in this temperature range. Combining ultra-low dissipation resonators with the very rich optical properties of TMD, paves the way for novel type of optomechanical experiments with 2D materials.

O 10.3 Mon 10:00 H16

Landau levels and Shubnikov-de Haas oscillations in monolayer transition metal dichalcogenide semiconductors — •Andor Kormányos[1], Péter Rakyta[2], and Guido Burkard[1] — [1]Physics Department, University of Konstanz — [2]Department of Theoretical Physics, Budapest University of Technology and Economics

We study the Landau level (LL) spectrum using a multi-band $\mathbf{k}\cdot\mathbf{p}$ theory in monolayer transition metal dichalcogenide semiconductors [1]. We find that in a wide magnetic field range the LL can be characterized by a harmonic oscillator spectrum and a linear-in-magnetic field term which describes the valley degeneracy breaking. The effect of the non-parabolicity of the band-dispersion on the LL spectrum is also discussed. Motivated by recent magnetotransport experiments, we use the self-consistent Born approximation and the Kubo formalism to calculate the Shubnikov-de Haas oscillations of the longitudinal conductivity. We investigate how the doping level, the spin-splitting of the bands and the broken valley degeneracy of the LLs affect the magnetoconductance oscillations. We consider monolayer MoS$_2$ and WSe$_2$ as concrete examples and compare the results of numerical calculations and an analytical formula which is valid in the semiclassical regime. Finally, we briefly analyze the recent experimental results [Cui et al., Nat. Nanotechnol. **10**, 534 (2015)] using the theoretical approach we have developed.

[1] New J. Phys. **17**, 103006 (2015).

O 10.4 Mon 10:15 H16

Second-harmonic generation in MoS2 monolayers coupled to resonant nanoantennas — •Franz Johannes Friedrich Löchner[1], Stefan Fasold[1], Antony George[2], Paul Douglas Harrison[1], Christoph Menzel[1], Andrey Turchanin[2], Isabelle Staude[1], Falk Eilenberger[3], Frank Setzpfandt[1], and Thomas Pertsch[1] — [1]Institute of Applied Physics, Abbe Center of Photonics , Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — [2]Institute of Physical Chemistry, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

Two-dimensional monolayers of transition metal dichalcogenides (TMDs), a new class of direct band-gap semiconductors, recently have attracted a lot of attention due to their pronounced excitonic emission lines and strong second-order nonlinearity.

Coupling TMDs to resonant nanoantennas allows to further enhance these effects by concentrating the exciting optical field into a small volume. Such enhancement has been shown for excitonic emission using plasmonic nanoantennas. However, nonlinear optical effects in TMD-nanoantenna systems have not been studied yet.

In our contribution, we report on experimental investigations of second-harmonic generation in molybdenum disulfide (MoS2) monolayers coupled to nanoantennas, resonant at the exciting fundamental-harmonic wavelength. Polarization resolved measurements show the profound impact which the presence of the nanoantenna has on the second-harmonic radiation generated by the MoS2-monolayer.

O 10.5 Mon 10:30 H16

Electrochemical growth and characterization of molybdenum sulfide layers for thin film transistors — •Talha Nisar, Torsten Balster, and Veit Wagner — Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany

Molybdenum disulfide has attracted considerable interest for its great potential in the field of nanoelectronics due to its semiconducting and 2D nature. It has been successfully deposited by the Scotch tape method resulting in high-mobility transistors with an area of a few square microns. The state-of-the-art method for the growth of crystalline molybdenum disulfide single and multilayers is chemical vapor deposition.

In our study we use electrochemical deposition as an alternative approach to grow large area molybdenum sulfide layers. For this purpose, ammonium tetrathiomolybdate (ATTM) has been used as precursor material for the electrodeposition in cathodic regime with respect to Ag/AgCl reference electrode. The obtained layers are amorphous as could be confirmed by Raman measurements. In addition, in the UV-VIS spectra of the MoS$_x$ (x=2..3) layer a transition at 2.4 eV is visible, which could be related to oxygen contamination. Further annealing steps in an Ar/H$_2$ atmosphere with an additional sulfur source at temperatures above 600°C are necessary to remove the oxygen and to convert the layer into crystalline MoS$_2$. The converted layer has to be transferred onto SiO$_2$/Si substrates for thin film transistor applications.

30 min. Coffee Break

Invited Talk O 10.6 Mon 11:15 H16

Epitaxial paradigms of van der Waals bonded chalcogenide materials — •Raffaella Calarco — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

In recent years it has become clear that materials with covalent bonding in only two dimensions (2D) have attractive properties for devices. The bonding in the third dimension, which is between individual layers, occurs by van der Waals (vdW) forces, which are weaker if compared to the covalent bonding. Materials used in conventional devices are instead characterized by covalent bonding in three dimensions (3D). In the present contribution, I shed some light on understanding the mechanisms that determine the interface structure between 2D and 3D or 2D materials. To study possible options for altering the bonding configurations of the 2D-3D interface GeTe-Sb2Te3 layers are deposited by molecular beam epitaxy on top of five different surface reconstructions-passivation of the Si(111). The 2D-2D interface is best studied using graphene as a substrate. Finally, I address the most crucial issue: The realization of vdW epitaxy in Sb2Te3-GeTe superlattices. Such superlattices, if compared to their alloy counterpart, show impressive performances highly attractive for future non-volatile memory applications.

O 10.7 Mon 11:45 H16

Transparent Conducting Materials: Insights from High-Throughput — •Pino D'Amico[1,2], Alice Ruini[1,2], Alessandra Catellani[2], Arrigo Calzolari[2], Marco Fornari[3,5], and Marco B. Nardelli[4,5] — [1]FIM-UNIMORE, Modena, Italy — [2]CNR-NANO S3, Modena, Italy — [3]Central Michigan Univ., Mt. Pleasant, USA — [4]Univ. of North Texas, Denton, USA — [5]Duke Univ., Durham, USA

Good electrical conductivity and optical transparency in the visible domain are the physical properties required in order to have Transparent Conducting Material (TCM). Various semiconductors becomes TCM when doped and up to now their discovery has followed an a-posteriori path: take a material and investigate its physical properties in order to see if it is a good TCM. Thanks to the large amount of data available in the AFLOWLIB repository[1], we use instead an inverse-design approach in order to search for new possible TCMs: starting from the paradigmatic case of ZnO[2] we have identified the physical descriptors representing a TCM and extracted from the database a list of materials having the required characteristics using highthroughput techniques. We investigated doped structures of resulting materials inserting substitutional elements in a systematic way with a given concentration. We will present an accurate study of both conductivity and optical properties of the doped structures obtained by means of a newly developed numerical tool based on Boltzmann theory and dielectric function calculations[3] and reliyng on an efficient ab-initio tight-binding representation of the lattice structures[4]. [1]www.aflowlib.org; [2]ACS Photonics 1, 703 (2014); [3]preprint(2015); [4]arXiv:1509.02558 (2015).

O 10.8 Mon 12:00 H16

Investigating the Potential of TMD Monolayers as Photodetectors — •Maja Feierabend[1], Gunnar Berghäuser[2], and Ermin Malic[2] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

Transition metal dichalcogenides (TMDs) are promising materials for technological application in the area of optoelectronics. Due to the direct band gap and the extraordinarily strong Coulomb interaction, TMDs exhibit efficient light-matter coupling and tightly bound excitons [1]. As atomically thin materials, they are very sensitive to changes in the surrounding environment. This motivates a functionalisation approach, where external molecules are non-covalently attached to the material surface to control its optical properties.

Here, we theoretically investigate functionalized TMDs based on the density matrix formalism combined with tight-binding wave functions. Considering exemplary spiropyran molecules exhibiting a strong dipole moment, we predict pronounced spectral red-shifts and the appearance of an additional side-peak in the absorption spectrum of functionalized TMDs. Interestingly, we also observe a further peak splitting due to the intervalley coupling between the high-symmetry K/K' points. The predicted pronounced changes in optical spectra of TMDs show their potential for technological application in photodetectors.

[1] G. Berghäuser and E. Malic, PRB 89, 125309 (2014)

O 10.9 Mon 12:15 H16

Investigation of excitonic resonances in monolayer MoSe2 for strong coupling experiments at room temperature — •Nils Lundt[1], Aleksander Maryński[2], Grzegorz Sek[2], Oliver Iff[1], Sefaattin Tongay[3], Sven Höfling[1,4], and Christian Schneider[1] — [1]Chair for Apllied Physics, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Physics, Wrocław University of Technology, Wybrzeze Wyspiańskiego 27, 50-370 Wrocław, Poland — [3]School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, Arizona 85287, United States — [4]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY 16 9SS, United Kingdom

We studied the temperature evolvement of the reflectivity of a MoSe2 monolayer. From this investigation we deduced the dependence of linewidth and oscillator strength on temperature. The results were used for transfer matrix simulations of strong coupling reflectivity spectra, expected if the MoSe2 monolayer is integrated into a micro-cavity. These calculations should evaluate, if strong coupling can be observed in MoSe2 monolayers at room temperature. Calculations were conducted for different cavity designs such as an open cavity approach, a monolithic cavity and for the coupling to a Tamm Plasmon. Moreover, we present results of excitation power dependent photoluminescence studies on MoSe2 monolayers.

O 10.10 Mon 12:30 H16

Localized states from WSe$_2$ as promising candidates for new single-photon sources — •Sven Borghardt[1], Jhih-Sian Tu[1], Florian Winkler[2], Detlev Grützmacher[1], and Beata Kardynal[1] — [1]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [2]ER-C, Forschungszentrum Jülich, Jülich, Germany

An emission of single photons from WSe$_2$ monolayers (ML) has been recently demonstrated but the origin of the emission is still not clear. The aim of our research is to understand its origin and then control the localized emission in this material to harvest the unique properties of the material for new applications in quantum photonics.

Samples prepared by exfoliation from synthetic crystals and also grown with CVD are measured using polarization resolved μ-photoluminescence (PL) as well as time-resolved PL.

Our results show linearly polarized emission doublet lines with an energy splitting of up to a few meV. The samples show a high density of such lines close to the sample edges. We attribute the linear polarization of the localized states to a mixing of K- and K'-states. There is an evidence of an alignment of the polarization of emission with the crystal lattice. PL from the localized states decays faster with the temperature than the one from the free exciton states. Chemical modification of the samples is further used in an attempt to manipulate the emission from the localized states.

O 10.11 Mon 12:45 H16

Theoretical studies of transition metal dichalcogenides for the use in electron holography — •Sven Borghardt[1], Zeila Zanolli[4], Matthieu Verstraete[3], Florian Winkler[2], Juri Barthel[2], Rafal Dunin-Borkowski[2], and Beata Kardynal[1] — [1]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [2]ER-C, Forschungszentrum Jülich, Jülich, Germany — [3]PCPM, Université Catholique de Louvain, Louvain-la-Neuve, Belgium — [4]PGI-2 and IAS, Forschungszentrum Jülich, Jülich, Germany

Few-layer transition metal dichalcogenides (TMDs) represent a new family of materials with promising properties for new optoelectronic nano-devices. Their well-known and tailorable thickness render them an ideal system for quantitative electron holography.

Here, we present the simulation of the effect of charge reorganisation due to bonding on the phase acquired by electrons passing through few layer TMD structures in electron holography experiments. This is done by simulating the phases for potentials from density functional theory calculations in comparison with ones obtained from the independent-atom approximation. The results show in an impressive way that neglecting the atomic bonding and the associated small change in the overall charge distribution leads to an overestimation of the average electron phase by approximately 5% for the analyzed materials. Comparison with experimental data confirms this conclusion.

Building on the results for pristine materials, we present calculations for single defects and heterostructures composed of different materials from the transtition-metal dichalcogenide family.

O 11: Plasmonics and Nanooptics II: Microscopy

Time: Monday 15:00–18:00 Location: S054

Invited Talk O 11.1 Mon 15:00 S054

Principles of plasmonic imaging — •Angela Demetriadou[1] and Alexei Kornyshev[2] — [1]Blackett Laboratory, Imperial College London, Prince Consort Road, SW7 2AZ, London, United Kingdom — [2]Department of Chemistry, Imperial College London, Prince Consort Road, SW7 2AZ, London, United Kingdom

Plasmonic imaging exploits the evanescent nature of propagating surface plasmon polariton (SPP) waves to produce real-time images of sub-wavelength objects with high-precision. It is commonly used in biological sciences to track and image organelles in cells, such as DNA, mitochondria and virus molecules. The fast dynamics of intra-cellular processes enforce to keep the cells under their native state (i.e. label-free) and to be imaged in real-time, establishing plasmonic imaging as a powerful tool for mapping and understanding cellular behaviour. Additionally, it has been widely used to map the electro-catalytic activity of single nanoparticles with high spatial resolution and sensitivity.

Our theoretical model describes the electromagnetic process that forms the plasmonic image, and accurately predicts the image properties for particles of any composition and size. The intensity and shape of the plasmonic image is dominated by the SPP-induced natural modes. Hence, through the theoretical model, spectroscopic information can be extracted from recorded plasmonic images, expanding the capabilities of current plasmonic imaging techniques.

O 11.2 Mon 15:30 S054

Imaging the dynamics of plasmonic vortices — •Deirdre Kilbane[1], Anna-Katharina Mahro[1], Stefan Mathias[1], Grisha Spektor[2], Lior Gal[2], Meir Orenstein[2], Bettina Frank[3], Simon Ristock[3], Harald Giessen[3], Philip Kahl[4], Daniel Podbiel[4], Frank Meyer zu Heringdorf[4], and Martin Aeschlimann[1] — [1]Physics Department and Research Centre OPTIMAS, University of Kaiserslautern, Germany — [2]Department of Electrical Engineering, Technion, Haifa, Israel — [3]Fourth Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [4]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

The formation of a plasmonic vortex (rotational flow around a phase singularity) can be achieved by selecting the spin of circularly polarized light, and the geometry of the illuminated metallic structure. We perform near-field imaging of the ultrafast dynamics of plasmonic vortices using time-resolved two photon photoemission electron microscopy (TR-PEEM). A broadband ultrashort pulse laser excites and probes surface plasmon polaritons (SPPs) with 100 as time step and 40 nm spatial resolution. Here we observe the sub-optical cycle spatiotemporal evolution of the dynamics in plasmonic Archimedes spirals (PAS) and plasmonic vortex lenses (PVL). These structures were fabricated by focused ion beam (FIB) milling into the surface of thin polycrystalline gold films and single crystalline, atomically flat gold flakes.

O 11.3 Mon 15:45 S054

Improving the lateral near-field confinement in a nanofocusing SNOM — •Simon F. Becker[1], Martin Esmann[1], KyungWan Yoo[1,2], Petra Gross[1], Ralf Vogelgesang[1], NamkYoo Park[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Seoul National University, Seoul, Korea

The lateral near-field confinement in apertureless scanning near-field optical microscopy (SNOM) experiments is typically governed by the tip radius of the probe used. Here, we discuss how to improve the confinement beyond this limitation using a nanofocusing SNOM taper.

We approach such a taper [1,2] to a thin, semitransparent gold film. Angle-resolved images of elastically scattered radiation transmitted through the film [3,4] show a steep increase in the detected signal over the last few nanometers. We compare the experimental results to finite element method simulations and find this steep increase to be a clear signature of gap plasmon formation in the gap between tip and sample. The lateral confinement of these fields is proportional to the geometric mean of tip-sample distance and tip radius. Hence, gap plasmons may enable decreasing the confinement to sizes typically found for interaction cross-sections of single quantum emitters. Combining this spectrally broadband effect with the background-free detection available with nanofocusing SNOM seems promising for nanospectroscopic investigations of dense and heterogeneous quantum emitter systems.

[1] M.I. Stockman, PRL 93, 137404 (2004); [2] S. Schmidt et al., ACS Nano 6, 6040 (2012); [3] M. Esmann et al., BJ Nano 4, 603 (2013); [4] S.F. Becker et al., (submitted).

O 11.4 Mon 16:00 S054

Coherent broadband nano-spectroscopy through plasmonic nanofocusing — •M. Esmann[1], S.F. Becker[1], H. Kollmann[1], J. Witt[1], K.W. Yoo[1,2], A. Chimeh[1], P. Gross[1], R. Vogelgesang[1], N.K. Park[2], and C. Lienau[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Seoul National University, Seoul, Korea

Plasmonic nanofocusing microscopy enables broadband coherent light scattering spectroscopy with 5 nm spatial resolution. This is used to image optical near-fields around individual metallic nanoparticles. Conceptually, surface plasmon polaritons are launched by a grating coupler on a conical metallic taper and propagate towards the taper apex where they are transformed into highly confined near-fields [1-3]. Upon optical interaction with a sample, far-fields scattered from the apex are collected almost background free. Here, we use coherent white light to excite this isolated, spectrally broadband nano-lightsource at the apex of a monocrystalline gold taper. We then investigate both the spectral and spatial characteristics of optical near-fields around chemically synthesized gold nanorods. We find dipolar plasmon resonances with comparatively high Q-factors of up to 15. These are confirmed by far-field measurements. We simultaneously also image the corresponding near-field pattern in the spatial domain and achieve spatial resolution down to 5 nm. As these measurements are fully coherent, they can be straightforwardly extended to the investigation of coherences in biological or semiconducting systems.

[1] M.I. Stockman, PRL 93, 137404 (2004); [2] S. Schmidt et al., ACS Nano 6, 6040 (2012); [3] M. Esmann et al., BJNANO 4, 603 (2013).

O 11.5 Mon 16:15 S054

Probing and Controlling Electronic and Vibrational Coherences in Individual Carbon Nanotubes using Femtosecond Pulse Shaping Microscopy — •Veit Giegold[1,2], Richard Ciesielski[1,2], Nicolai F. Hartmann[3], Erik H. Haroz[3], Stephen K. Doorn[3], and Achim Hartschuh[1,2] — [1]Department Chemie and CeNS, LMU Munich, 81377 Munich — [2]Nanosystems Initiative Munich, 80799 Munich — [3]Los Alamos National Laboratory, New Mexico, 87545 United States

We probe and coherently manipulate the exciton population of individual semiconducting single-walled carbon nanotubes (SWCNTs) at room temperature using femtosecond laser pulse shaping microscopy [1,2]. In our experiment, the exciton state E_{11} of defect-doped (5,4)-SWCNTs is resonantly excited by a pair of phase-locked 20 fs laser pulses while the photoluminescence (PL) emission of the defect state E_{11}^{D} serves as reporter for the E_{11}-population. Tuning the pulse delay and relative carrier envelope phase results in damped PL intensity oscillations that can be described using the Bloch equations for a two-level system. We show that light absorption of individual SWCNTs can be controlled within their electronic dephasing time, ranging from 20 to 66 fs for different nanotubes. For longer pulse separations coherent radial breathing mode excitations with a period of 90 fs are observed.

[1] R. Hildner, D. Brinks, N.F. van Hulst, Nature Physics (2010).

[2] R. Ciesielski, V. Giegold, A. Hartschuh, et al., in prep.

O 11.6 Mon 16:30 S054

Confocal active interference scattering microscopy: A new approach to characterize single gold nanoparticles — •Otto Hauler — Institute of Physical Chemistry — Tübingen — Germany

Gold nanoparticles and their applications have attracted considerable research interest in recent times. By using confocal interference microscopy in combination with cylindrical vector beams it is possible to directly image the orientation and to detect the shape of single metal nanoparticles, with sizes well beyond the diffraction limit [1-4]. We present a newly developed method to further investigate the properties of these promising materials, the confocal active interference scattering microscope. This novel technique allows the measurement of the phase of the elastically scattered light. It furthermore enables the control of the excitation polarization, through the use of radially- and azimuthally-polarized laser modes. [1] A.V. Failla, H. Qian, H. Qian, A. Hartschuh, A. J. Meixner, Nano Lett. (2006), 6: 1374. [2]

F. Wackenhut, A.V. Failla, A.J. Meixner, Phys. Chem. Chem. Phys. (2013),15: 5407-5414. [3] F. Wackenhut, A.V. Failla, A.J. Meixner, Anal Bioanal Chem (2015), 407: 4029-4034. [4] F. Wackenhut, A.V. Failla, T. Züchner, M. Steiner, A.J. Meixner, Appl. Phys. Lett. (2012), 100: 263102.

O 11.7 Mon 16:45 S054

Polarization sensitive scanning near field optical microscope on polymer thin films — •Jens Brauer[1], Jinxin Zhan[1], Petra Gross[1], Christoph Lienau[1], Daniel Trefz[2], and Sabine Ludwigs[2] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Institut für Polymerchemie, Stuttgart, Germany

Currently there is a high need to investigate the relationship between structure and functionality of novel, polymer-based organic solar cell materials. Specfically information about local fluctuations of their optical properties, largely affecting the charge carrier mobility is needed [1]. For this, an optical imaging method is required with a spatial resolution in the order of the domain size, typically a few nanometers, or even below.

Here we present a technique to use near field optical microscopy to fulfill these requirements. We use a Titanium:Sapphire laser focused through the sample onto a sharp gold tip and collect the scattered near-field signal from the tip in a backscattering geometry. By applying a modulation to the tip with tens of kilohertz and using a lock-in amplifier after detection to demodulate the signal at the n-th harmonic we can significantly increase the signal to noise ratio. Changing the direction of the linear laser polarization enables us to determine the molecular orientation with a resolution of about 10 nm. In this talk we present a first demonstration by applying the technique to ordered and unordered thin film polymer samples.

[1] Brinkmann, M. et al.; ACS Nano 6, pp 10319-10326 (2012)

O 11.8 Mon 17:00 S054

Nanoscale probing of optical near-fields by ultrafast transmission electron microscopy — •Armin Feist, Katharina E. Echternkamp, Murat Sivis, Sascha Schäfer, and Claus Ropers — 4th Physical Institute, University of Göttingen, Göttingen, Germany

Ultrafast transmission electron microscopy (UTEM) allows for the study of structural and electronic dynamics on nanometer length scales [1], as well as for the local probing of optical near-fields [2].

Here, we employ the inelastic scattering of swift electrons to characterize optical near-fields in metallic nanostructures. The experiments utilize a novel short-pulsed electron gun driven by localized photoemission from a nanotip emitter, yielding electron probes with a pulse duration of 300 fs and beam diameters down to 1.5 nm.

In the interaction with optical near-fields, the energy spectra of free electrons develop into a comb of spectral sidebands representing the absorption and emission of multiple photons [2]. The quantum coherence of this process is evidenced by the observation of multilevel Rabi oscillations in the sideband populations [3]. The interaction facilitates few nanometer spatial resolution in near-field imaging, as demonstrated by raster-scanning the focused electron probe across resonantly excited plasmonic nanostructures with feature sizes down to 5 nm.

[1] A.H. Zewail, Science, **328**, 187 (2010).
[2] B. Barwick *et al.*, Nature, **462**, 902 (2009).
[3] A. Feist *et al.*, Nature, **521**, 200 (2015).

O 11.9 Mon 17:15 S054

Coherent spectroscopy of single metallic nanostructures — •Martin Silies[1], Heiko Kollmann[1], Martin Esmann[1], Julia Witt[2], Gunther Wittstock[2], and Christoph Lienau[1] — [1]AG Ultraschnelle Nano-Optik, Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]AG Wittstock, Institut für Chemie, Carl von Ossietzky Universität Oldenburg, Germany

Metallic nanostructures exhibit strong optical resonances and enhanced optical near-fields, enabling the transfer of far-field radiation onto subwavelength scales. Even so, the mismatch of the optical absorption or scattering cross-section of a single nanostructure and the free space wavelength makes far-field spectroscopic investigations challenging. Further, single nanostructures with geometric dimensions of less than 50nm require highly sensitive and almost background-free spectroscopic methods. For this, modulation-based methods such as focus or Spatial Modulation Spectroscopy (SMS)[1] have been proven to be able to quantitatively measure the scattering and absorption cross section simultaneously [2]. Here, we present a combined approach of a commonly used confocal SMS setup and broadband VIS-IR Fourier Transform spectroscopy to measure the extinction cross section of single nanostructures in the time domain. We show polarization-resolved spectra of single chemically synthesized gold nanorods resonant in the near infrared. An extension of the approach to the study of hybrid nanostructures and to time-resolved phenomena is discussed.

[1] A. Arbouet et al., PRL 93, 127401 (2004)
[2] M. Husnik et al., PRL 109, 233902 (2012)

O 11.10 Mon 17:30 S054

Plasmon-mediated circularly polarized luminescence of GaAs in a scanning tunneling microscope — Svenja Mühlenberend, Markus Gruyters, and •Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

The electroluminescence from *p*-type GaAs(110) in a scanning tunneling microscope has been investigated at 6 K. Unexpectedly high degrees of circular polarization have often been observed with ferromagnetic Ni tips and also with paramagnetic W and Ag tips. The data is interpreted in terms of two distinct excitation mechanisms. Electron injection generates intense luminescence with low polarization. Plasmon-mediated generation of electron-hole pairs leads to less intense emission, which, however, is highly polarized for many tips.

O 11.11 Mon 17:45 S054

Plasmonic Activation of Platinum Clusters for Photocatalytic Reactions Detected by STM — Sarah Wieghold[1], Lea Nienhaus[2,3], Marian D. Rötzer[1], Fabian Knoller[1], Florian F. Schweinberger[1], Joseph W. Lyding[2], Ulrich Heiz[1], Martin Grübele[2,3], and •Friedrich Esch[1] — [1]Chemistry Dept. and CRC, TU München, Lichtenbergstr. 4, 85748 Garching, Germany — [2]Beckman Institute, University of Illinois, Urbana — [3]Department of Chemistry, University of Illinois, Urbana, Illinois 61801

Their unique structural, optical and electronic properties make small metal clusters prime candidates for catalytic applications, especially under mild reaction conditions such as in photocatalysis. Due to their small cross sections for the interaction with light and due to low surface coverages, an indirect, support-mediated photoactivation mechanism is most efficient. We imaged this activation at the level of individual $Pt_{>35}$ clusters supported on a thin, structured gold film. The film shows a strong plasmonic interaction with visible light that is optimized to work in a back-illumination geometry. We used a scanning tunneling microscope to map the tunneling current modulation induced by light at 532 nm. When tunneling into unoccupied states of the film, we detect a light-induced current increase that is enhanced on the clusters. In this way, we image the plasmonic coupling of the clusters to the gold support with nanometer resolution. This activation leads indeed to an enhanced catalytic activity, as we demonstrate for the oxidative decomposition of methylene blue.

O 12: Morphology Prediction at Interfaces

Time: Monday 15:00–18:30 Location: S051

O 12.1 Mon 15:00 S051

Flexible 2D crystals of polycyclic aromatics stabilized by static distortion waves — Matthias Meissner[1], Falko Sojka[1], Lars Matthes[2], Friedhelm Bechstedt[2], Xinliang Feng[3], Klaus Müllen[3], Stefan C. B. Mannsfeld[4], •Roman Forker[1], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany — [2]Institute of Condensed Matter Theory and Solid State Optics, Friedrich Schiller University Jena, Germany — [3]Max Planck Institute for Polymer Research, Mainz, Germany — [4]Center for Advancing Electronics, TU Dresden, Germany

The epitaxy of many organic films on inorganic substrates can be classified by established lattice match conditions. Yet, there are material-substrate combinations for which this classification fails and cannot be exploited to understand reproducible azimuthal alignments between adsorbate and substrate lattices. For decades it has been hypothesized in the literature that so-called static distortion waves (SDWs) could be responsible for the observed orientational epitaxy in such cases. By means of STM and LEED experiments we demonstrate unequivocally SDWs in films of hexa-*peri*-hexabenzocoronene on graphite, which manifest as sub-Ångström local molecular displacements from an ideal rigid adsorbate lattice, being itself *incommensurate* with graphite in contrast to previous reports. We present a model that consistently explains these displacements in both size and direction. Based on DFT we calculate for realistically large domains the energy gain due to the SDWs, thereby proving their crucial role for the observed epitaxy, and we successfully reproduce the measured domain angle.

O 12.2 Mon 15:15 S051

Structural properties of picene-perfluoropentacene and picene-pentacene blends: Superlattice formation versus limited intermixing — J. Dieterle[1], K. Broch[1,2], A. Hinderhofer[1], H. Frank[1], J. Novák[3], •A. Gerlach[1], T. Breuer[4], R. Banerjee[1], G. Witte[4], and F. Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Cavendish Laboratory, University of Cambridge, UK — [3]Central European Institute of Technology, Masaryk University, Czech Republic — [4]Fachbereich Physik, Philipps-Universität Marburg, Germany

The structure and morphology of mixed thin films of picene ($C_{22}H_{14}$, PIC) and perfluoropentacene ($C_{22}F_{14}$, PFP) as well as mixed thin films of PIC and pentacene ($C_{22}H_{14}$, PEN) grown by simultaneous coevaporation is investigated using X-ray diffraction, atomic force microscopy, and near-edge X-ray absorption spectroscopy. For both systems we find mixing on the molecular level and the formation of mixed structures. However, due to the strongly different interactions in both mixtures the ordering is fundamentally different [1]. The results are discussed in the context of other organic semiconductor binary mixtures [2] showing that besides chemical composition and steric compatibility the intramolecular arrangement of the atoms important for intermolecular interactions significantly influences the structure formation in organic semiconductor blends.

[1] J. Dieterle et al., J. Phys. Chem. C **119** (2015) 23211.
[2] C. Lorch et al., Appl. Phys. Lett. **107** (2015) 201903.

O 12.3 Mon 15:30 S051

Exploring the Electronic and Vibrational Properties of Disordered TCNE on Cu(111) Using a Basin Hopping Algorithm — •Veronika Obersteiner, Egbert Zojer, and Oliver T. Hofmann — Instiute of Solid State Physics, NAWI Graz, Graz Univeristy of Technology, Austria

While to date most first-principle studies focus on highly ordered crystalline materials, in this work we concentrate on the theoretical investigation of amorphous or disordered materials that are commonly used in experimental applications. To sample the complex potential energy surface (PES) of disordered organic/inorganic interfaces we develop a three-step geometry search algorithm based on Basin Hopping (BH) in conjunction with dispersion-corrected Density Functional Theory. First, we determine the local adsorption structures, then we coarse-grain the PES as a superposition of these local adsorption structures to finally efficiently jump between the locally optimized configurations using the BH algorithm.

Applying this approach to TCNE (tetracyanoethene) on Cu(111) we evaluate a set of energetically lowest lying structures, reflecting the distribution of local conformations and their environment. Our investigations reveal that at finite temperature a noticeable amount of TCNE molecules are bound in an upright standing manner to the Cu(111) surface, although this is not the global minimum. The different adsorption conformations exhibit very different electronic properties characterized by the charge states of the TCNE molecules and their vibrational spectra.

O 12.4 Mon 15:45 S051

Machine learning of surface adsorbate structure — •Milica Todorović[1], Michael Gutmann[2], Jukka Corander[2], and Patrick Rinke[1] — [1]Aalto University, Espoo, Finland — [2]University of Helsinki, Helsinki, Finland

To efficiently search many atomistic configurations on large length scales, we developed a parameter-free machine learning tool for studying organic/inorganic interfaces. Our preferred Bayesian optimisation approach relies on probabilities to construct model functions, which are then iteratively refined by input of real data points balancing exploitation with exploration. A Bayesian optimisation algorithm was interfaced with both classical potential and density-functional theory codes to enable iterative learning (on-the-fly) of potential energy surfaces (PES) on large supercomputers without human input. For additional efficiency, the method exploits structural rigidity of molecular groups, reducing the degrees of freedom and making the learning process analogous to "molecular LEGO". We present a proof-of-concept test based on the alanine molecule and an application featuring electron donor C_{60} molecules on the (101) surface of TiO_2 anatase. The Bayesian optimisation structure search (BOSS) acquires PES information fast and is particularly efficient in pinpointing the global minimum structure. This versatile scheme for global minimum search could be extended beyond interface packing considerations to address complex configurational problems across scientific disciplines.

O 12.5 Mon 16:00 S051

Substrate-Induced Phases: Polymorphism of Organic Materials on Surfaces — •Andrew O. F. Jones[1], Basab Chattopadhyay[2], Yves H. Geerts[2], and Roland Resel[1] — [1]Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Laboratoire de Chimie des Polymères, Faculté des Sciences, Université Libre de Bruxelles CP206/01, Campus de la Plaine, 1050 Brussels, Belgium

An increase or change of structural order in the vicinity of a solid substrate is known for a wide variety of materials. For molecular materials crystallizing on a solid surface, it has been observed that new polymorphic forms may exist near the interface with the substrate which have structures markedly different to those observed in the bulk material; such phases are termed Substrate-Induced Phases (SIPs). [1] The presence of a SIP in a compound or a class of materials can be of crucial significance in terms of its physical properties. However, the factors that drive such a process are not clearly understood or studied in depth. With the ultimate aim of controlling material properties by controlling structure, it is essential to take account of changes in the structure brought about by SIPs and to work towards controlling polymorphism in organic thin films. Several examples, with a particular focus on organic semiconducting materials, will be discussed to highlight the types of materials that can display SIPs and the current understanding of their origins.

[1] A. O. F. Jones, B. Chattopadhyay, Y. H. Geerts, R. Resel, Adv. Funct. Mater., 2015, Accepted for Publication.

O 12.6 Mon 16:15 S051

In-situ LEEM study of the growth of NTCDA on Cu(001) — •Jana Wolters, Janina Felter, Markus Franke, Caroline Henneke, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology, Germany

A good understanding of the interactions between organic molecules and metal surfaces is essential for improving the performance of organic (opto-) electronic devices as well as for fundamental studies of thin organic films and metal-organic interfaces. In this context the first organic layer adsorbed on the metal substrate is of special importance since it is serving as a template for further growth and directly influences the physical properties of the interface.

As a model system, we investigated the growth of 1,4,5,8-naphthalene-tetracarboxylic-dianhydride (NTCDA) on the Cu(001)-surface in-situ and in real-time with LEEM, and correlated the results with structural information obtained by μLEED. We identified several different phases occurring at different temperatures. For one of them, we observed an unexpected behavior that resembles dendritic growth.

O 12.7 Mon 16:30 S051

Long-Range Order Induced by Intrinsic Repulsion on an Insulating Substrate — Julia L. Neff[1], Hagen Söngen[1], •Ralf Bechstein[1], Philipp Maass[2], and Angelika Kühnle[1] — [1]Institute of Physical Chemistry, Johannes Gutenberg University Mainz, Duesbergweg 10-14, 55099 Mainz, Germany — [2]Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück, Germany

Creating complex functional structures on surfaces requires tools like molecular self-assembly. Here, adjusting the balance between intermolecular and molecule-surface interactions is a versatile strategy for tailoring molecular structure formation. Short-ranged attractive forces have often been in the focus while long-ranged repulsive interactions have been explored only rarely, despite their potential for steering molecular order formation. We report an ordered arrangement of molecular stripes with equidistant appearance that is formed upon the adsorption of 3-hydroxybenzoic acid onto calcite (10.4) at room temperature. The observed next-neighbor stripe distance distributions deviate substantially from random distributions of non-interacting stripes, verifying the existence of a repulsive interaction between the stripes. Even at low molecular coverage, where the average stripe distance is as large as 16 nm, the stripes are significantly ordered, demonstrating the long-range nature of the involved repulsive interaction. We show, it is plausible that adsorption-induced charge redistribution alone is responsible for the observed long-range repulsion. This generic repulsion mechanism is expected to play an important role in molecular self-assembly on insulators.

O 12.8 Mon 16:45 S051

Interface formation of aromatic molecules on a metal/metal-oxide nano-template mediated by lateral and vertical interactions — •Alexander Timmer, Harry Mönig, Oscar Díaz Arado, Saeed Amirjalayer, Martin Uphoff, and Harald Fuchs — Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

The self-assembly of organic molecules on pre-structured surfaces is a promising approach to steer precise arrangement of molecular nanostructures. The Cu(110)-(2x1)-O added row reconstruction of a partially oxidized Cu(110) surface, where added Cu and O atoms are arranged in a striped super-grating along the [100] direction, forms an interesting nano-template exhibiting a well-defined lateral metal/metal-oxide phase boundary. Previous studies showed that various organic compounds exclusively adsorb on the pure metal domains. By STM imaging we confirm this finding for different polycyclic aromatic hydrocarbons. For low coverages, these molecules predominantly decorate the metal/metal-oxide boundaries of the (2x1)-O strings in a specific geometry. By constant height NC-AFM imaging with an O-terminated Cu tip we achieve both sub-molecular resolution and chemical identification within the oxide reconstruction allowing a precise adsorption site determination. Supported by DFT calculations the adsorption behavior adjacent to the Cu(110)-(2x1)O reconstruction is compared to the adsorption on the Cu(110) surface, providing a conclusive picture of the fine interplay between the involved lateral and vertical interaction.

O 12.9 Mon 17:00 S051

Interaction of free-base tetraphenyl porphyrin with MgO(001) surface — •Osman Barış Malcioğlu[1] and Michel Bockstedte[1,2] — [1]Lehrstuhl f. Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]Chemie und Physik der Materialien, Universität Salzburg, Salzburg, Austria

MgO(001) as a pristine surface is chemically rather inert. Under experimental conditions, step edges, kink-sites and other low coordinated sites are present. Such sites may chemically interact with adsorbates and hence play a role in structure formation. Recently, the metalation of H2TPP with Mg via low coordinated sites on MgO(001) has been demonstrated [1]. The mechanisms underlying this processess, however, remain unclear. We employ ab-initio molecular dynamics simulations to study how H2TPP may interact with MgO(001) and common low coordinated sites. We find that H2TPP is mobile on the pristine surface since the phenyl rings stericly hinder physisorption at a specific surface site. In the presence of a step or kink site, however, phenyl rings help form a rather stable complex. The molecule aligns at the step or kink such that spontaneous deprotonation of the macrocycle occurs. We present the electronic and structural properties of the adsorbate complex and investigate the photophysical fingerprint of intermediates and the metallized porphyrins using (hybrid) TDDFT, self consistent GW and BSE.

[1] J. Schneider *et al.*, ACS Appl. Mater. Interfaces 7, 22962 (2015).

O 12.10 Mon 17:15 S051

Temperature dependence of ethanol water nanophase separation in soft graphene mica slitpore — •Abdul Rauf[1], Jonas Gienger[2], Nikolai Severin[1], Igor M. Sokolov[1], and Jürgen P. Rabe[1,3] — [1]Humboldt Universität zu Berlin — [2]Physikalisch-Technische Bundesanstalt, Berlin — [3]IRIS Adlershof, Berlin

Real space imaging with Scanning Force Microscopy (SFM) revealed nanophase separation in a fluid monolayer of ethanol and water confined in a soft graphene-mica slitpore. The interactions which determine the irregular equilibrium patterns had been attributed qualitatively to the interplay of short-range attractive, and long-range electrostatic repulsive interactions. However, determining strength and range of these interactions quantitatively presented a challenge due to the complex screened dipole-dipole interactions, the bending energy of the graphene sheet, and intermolecular interactions. The interaction potential, however, has been reconstructed applying an Inverse Monte Carlo approach on SFM micrographs of the system. The reconstructed potential was then used to predict the behavior of the system outside the experimentally accessible range of parameters such as temperature and vapor pressure, including critical demixing temperature. [1]

To validate this approach experimentally, its predictions regarding the response of the system to temperature changes were tested by imaging the nanophase-separated patterns at various temperatures using an SFM equipped with heating/cooling elements. [1] J. Gienger, N. Severin, J. P. Rabe, I. M. Sokolov 2015, arXiv:1505.03011 [cond-mat.stat-mech]

O 12.11 Mon 17:30 S051

An Interfacial Bridge from a Perovskite to a Fluorite — Marita O'Sullivan[1], Joke Hadermann[2], •Matthew S Dyer[1], Stuart Turner[2], Jonathan Alaria[1], Troy Manning[1], Artem M Abakumov[2], John B Claridge[1], and Matthew J Rosseinsky[1] — [1]University of Liverpool, Liverpool, UK — [2]EMAT, Univerisity of Antwerp, Antwerp, Belgium

Coherent interfaces between materials are essential for many technological processes, and can give rise to novel physical properties. Such interfaces can be obtained by controlled 2D layer-by-layer growth of one material on another. Dimensional matching on the unit cell length scale can usually used to determine whether 2D layer-by-layer growth is possible when both materials have the same or similar structures, but not when the materials have very different structures. For example, perovskite / fluorite interfaces can be engineered with less than 1 % strain, but 2D layer-by-layer growth still cannot be achieved. Using pulsed laser deposition, we demonstrate 2D layer-by-layer growth of the lattice matched disordered fluorites $La_{0.5}Zr_{0.5}O_{1.75}$ and $Nd_{0.5}Zr_{0.5}O_{1.75}$ on the perovskite $LaAlO_3$. A joint DFT and STEM investigation of the interface shows that local restructuring occurs forming a bridge between the perovskite and fluorite, satisfying the local bonding of both structures. The restructuring is made possible by the chemical flexibility of the chosen fluorites. This suggests both dimensional and chemical matching are important for the creation of coherent interfaces between materials with significantly differing structures, and that chemical mismatches can be overcome by a careful choice of materials.

O 12.12 Mon 17:45 S051

Hydroxylation and segregation induced morphology changes of MgO cube based nanostructures — Daniel Thomele[1], Andreas Sternig[2], Johannes Bernardi[3], Simon Klacar[4], Henrik Grönbeck[4], and •Oliver Diwald[1] — [1]Department of Chemistry and Physics of Materials, University of Salzburg, Salzburg, Austria — [2]Institute of Particle Technology, University of Erlangen-Nürnberg, Erlangen, Germany — [3]University Service Center of Transmission Electron Microscopy, TU Vienna, Austria — [4]Department of Applied Physics and Competence Centre for Catalysis, Chalmers University of Technology, Göteborg, Sweden

Vapor phase grown MgO cubes have turned out to be extremely valuable probes for the investigation of interface chemistry and particle morphology evolution inside powders. Comparative annealing experiments on these materials in dynamic high vacuum and in different gas atmospheres revealed the dramatic impact of residual water and surface hydroxylation on particle morphology and sintering properties. Moreover, we investigated the structural and energetic properties of Barium oxide (BaO) units dissolved inside the MgO host and adsorbed on MgO particle surfaces with HR Transmission Electron Microscopy and Density Functional Theory (DFT) calculations. The shape of BaO and MgO particles in a water environment were investigated as a function of temperature. The calculations suggest that the spherical shapes of the segregates result from the growth process and become thermodynamically stabilized by surface hydroxylation.

O 12.13 Mon 18:00 S051

Probing the interface between semiconducting nanocrystals and molecular metal chalcogenide surface ligands: insights from *first principles*. — Emilio Scalise[1], Stefan Wippermann[1], Giulia Galli[2], and •Dmitri Talapin[2] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]University of Chicago, Chicago, United States

Colloidal nanocrystals (NCs) are emerging as cost-effective materials offering exciting prospects for solar energy conversion, light emission and electronic applications. Recent experimental advances demonstrate the synthesis of fully inorganic nanocrystal solids from chemical solution processing. The properties of the NC-solids are heavily determined by the NCs surface and their interactions with the host matrix, due to the high surface-to-volume ratio. However, information on the atomistic structure of such composites is hard to obtain, due to the complexity of the synthesis conditions and the unavailability of robust experimental techniques to probe nanointerfaces at the microscopic level. Here we present a systematic theoretical study of the interaction between InAs and InP NCs with $Sn_2S_6^{4-}$ ligands. Employing a grand canonical *ab initio* thermodynamic approach we investigate the relative stability of a multitude of configurations possibly realized at the NC-ligand interface. Our study highlights the importance of different structural details and their strong impact on the resulting composite's properties. We show that to obtain a detailed understanding of experimental data it is necessary to take into account complex interfacial structures beyond simplified NC-ligand model interfaces.

O 12.14 Mon 18:15 S051

A research concept for understanding morpology evolution and nanoscale atomic arrangement in multicomponent thin films — Viktor Elofsson[1], Georgios Almyras[1], Bo Lü[1], Robert Boyd[2], and •Kostas Sarakinos[1] — [1]Nanoscale Engineering Division, Department of Physics, Chemistry and Biology, Linköping University, SE-58183, Linköping, Sweden — [2]Plasma and Coatings Physics Division, Department of Physics, Chemistry and Biology, Linköping University, SE-58183, Linköping, Sweden

Synthesis of multicomponent thin films using vapor fluxes with a modulated deposition pattern is a potential route for accessing a wide gamut of atomic arrangements and morphologies for property tuning. In the current study, we present a research concept that allows for understanding the combined effect of flux modulation, kinetics and thermodynamics on the growth of multinary thin films. This concept entails the combined use of thin film synthesis by means of multiatomic vapor fluxes modulated with sub-monolayer resolution, deterministic growth simulations and nanoscale microstructure probes. Using this research concept we study structure formation within the archetype immiscible Ag-Cu binary system showing that atomic arrangement and morphology at different length scales is governed by diffusion of near-surface Ag atoms to encapsulate 3D Cu islands growing on 2D Ag layers. The knowledge generated and the methodology presented herein provides the scientific foundation for tailoring atomic arrangement and physical properties in a wide range of miscible and immiscible multinary systems.

O 13: Magnetic Surface Excitations

Time: Monday 15:00–17:30 Location: S052

Invited Talk O 13.1 Mon 15:00 S052

Excitations and dynamics of non-collinear magnetization states in tailored adatom arrays — •Jens Wiebe — Department of Physics, Universität Hamburg, D-20355 Hamburg, Germany

Arrays of magnetic atoms adsorbed on the surface of a non-magnetic metal can be tailored in topology [1], magnetic anisotropy [2,3], interactions [1,4], and Kondo coupling [3] by combining different substrate/adatom species with the manipulation- [1], spin-resolved- [5] and inelastic- [6] spectroscopy capabilities of the scanning tunneling microscope. Such arrays are perfect model systems to study the complex phase diagram of strongly correlated multi-orbital electron systems. Here, I will focus on the rich physics we recently discovered in arrays of iron adatoms on platinum(111) [2,3,7]. This system can be theoretically described within the Hund's metal framework. We can tune the individual constituents, the Hund's impurities, from a regime of emergent magnetism to a multi-orbital Kondo state [3]. By coupling a few Hund's impurities to arrays, we find non-collinear ground states induced by the substrate mediated Ruderman-Kittel-Kasuya-Yosida interaction [7]. I will present our investigation of the excitations and dynamics of such non-collinear magnetization states.

[1] A. A. Khajetoorians *et al.*, Nat. Phys. **8**, 497 (2012). [2] A. A. Khajetoorians *et al.*, PRL **111**, 157204 (2013). [3] A. A. Khajetoorians *et al.*, Nat. Nano. **10**, 958 (2015). [4] L. Zhou *et al.*, Nat. Phys. **6** 187 (2010). [5] J. Wiebe *et al.*, JPD **44**, 464009 (2011). [6] A. A. Khajetoorians *et al.*, Nature **467**, 1084 (2010). [7] A. A. Khajetoorians *et al.*, Nat. Comm., (accepted, 2015).

O 13.2 Mon 15:30 S052

Origin of inelastic excitations in rare-earth based metal-organic complexes — •Daniela Rolf[1], Matthias Bernien[1], Paul Stoll[1], Qingyu Xu[1], Fabian Nickel[1], Claudia Hartmann[1], Tobias R. Umbach[1], Jens Kopprasch[1], Janina N. Ladenthin[1], Enrico Schierle[2], Eugen Weschke[2], Constantin Czekelius[3], Wolfgang Kuch[1], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [3]Heinrich-Heine-Universität Düsseldorf, Germany

Rare-earth atoms with a partially filled f shell exhibit interesting magnetic properties due to their large magnetic anisotropy. Within the Dysprosium-tris(1,1,1-trifluoro-4-(2-thienyl)-2,4-butanedionate) ($Dy(tta)_3$) complex, Dy exhibits a total angular momentum of J = 15/2 with anisotropy-split M_J levels. Employing low-temperature STM we show that deposition of $Dy(tta)_3$ on a Au(111) surface leads to densely packed self-assembled islands. XMCD measurements on $Dy(tta)_3$ show a sizeable magnetic anisotropy. dI/dV-spectra on these molecules exhibit symmetric steps at ±7.6 meV, which correspond to an inelastic excitation. To identify the origin of this feature unambiguously, we compare to spectra taken on the isostructural $Gd(tta)_3$, showing an inelastic step at a similar energy. As Gd^{3+} has a half-filled f shell, it is not expected to show any magnetic anisotropy. Hence, we conclude that the inelastic steps do not arise due to transitions between the anisotropy-split spin states, but can be explained by the excitation of molecular vibrations.

O 13.3 Mon 15:45 S052

Tuning the Kondo coupling strength of a single molecule — •Olof Peters[1], Benjamin W. Heinrich[1], Christian Lotze[1], Xianwen Chen[1], Markus Ternes[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Max-Planck Institut for Solid State Research, Stuttgart, Germany

Metal adatoms on a metal surface are typically strongly Kondo coupled, leading to a high Kondo temperature T_K, whereas insulating films efficiently reduce the coupling of such adsorbates resulting in much lower T_K. This decoupling gives the opportunity to study the Kondo effect with today's accessible magnetic fields and temperature ranges. A disadvantage of these isolating layers is the fixed coupling constant determined by the specific system.

We report on the controllable, continuous and reversible tuning of the Kondo coupling between a metal-organic complex (Fe-octaethylporphyrin-Cl) and its underlying Au(111) metal surface under the influence of a scanning tunnelling microscope tip at 1.1 K. Upon approach of the STM tip to the Fe core, the magnetic anisotropy increases and eventually a Kondo resonance appears. The Kondo coupling strength continuously increases at further tip approach.

We ascribe these results to a modification of the crystal field by the tip leading to a shift in the d-level energies. The change in crystal field also results in a relaxation of the Fe atom towards the substrate thus tuning the magnetic interactions from weak into the strong Kondo coupling regime.

O 13.4 Mon 16:00 S052

Reversible switching of the Kondo effect at a giant Rashba surface — •Jens Kügel, Andreas Krönlein, and Matthias Bode — Experimentelle Physik II, Würzburg, Germany

Transition metal phthalocyanine (TMPc) molecules on metal substrate have recently attracted considerable interest, as they offer a versatile platform to study and the tune magnetic interaction of the central metal ion with the substrate's conduction electrons [1,2]. Especially the Kondo effect arising from unscreened magnetic moments of the metal ion has been intensively studied [3,4].

In this contribution we present a low-temperature ($T = 5\,K$) scanning tunneling microscopy and spectroscopy (STS) study of single MnPc molecules adsorbed on $BiAg_2$, a surface alloy which has been shown to exhibit a giant Rashba effect [5]. We will show that a STS feature close to the Fermi energy —most likely a signature of Kondo screening— can be reversible switched on and off by controlled manipulation with the STM tip.

[1] A. Zhao *et al.*, Science **309**, 1542 (2005).
[2] J. Kügel *et al.*, Phys. Rev. B **91**, 235130 (2015).
[3] D. Rakhmilevitch *et al.*, Phys. Rev. Lett. **113**, 236603 (2014).
[4] A. Strozecka *et al.*, Phys. Rev. Lett. **109**, 147202 (2012).
[5] C. R. Ast *et al.*, Phys. Rev. Lett. **98**, 186807 (2007).

O 13.5 Mon 16:15 S052

Tailoring the magnetic ground state of a two-molecule Kondo system by chemical interactions — •T. Esat[1], B. Lechtenberg[2], T. Deilmann[3], C. Wagner[1], P. Krüger[3], R. Temirov[1], M. Rohlfing[3], F.B. Anders[2], and F.S. Tautz[1] — [1]Peter Grünberg Institute (PGI-3), FZ Jülich, Germany — [2]Institut für Festkörpertheorie, Universität Münster, Germany — [3]Lehrstuhl für Theoretische Physik II, TU Dortmund, Germany

Molecules are considered to be a promising platform for spintronics since self-assembly offers the opportunity to create tailored arrays of single spins. In this context, engineering the interaction between spins is crucial for future applications.

Rather than relying on the magnetic exchange interaction to tailor the magnetic properties of a nanostructure, we propose a novel approach to achieve the same goal: it relies on the systematic use of the ubiquitous non-magnetic chemical interaction between the constituents of the nanostructure. Our approach is crucially based on spin-moment carrying orbitals that are extended in space [1] and therefore allow the direct coupling of magnetic properties to wave function overlap, i.e. the formation of chemically bonding and anti-bonding orbitals. We demonstrate the approach for a dimer of metal-molecule complexes on the Au(111) surface. Changing the wave function overlap between the two monomers, we tune the dimer through a quantum phase transition from a triplet to a singlet ground state, with one configuration being located extremely close to a quantum critical point.

[1] T. Esat et al., Phys. Rev. B 91, 144415 (2015)

O 13.6 Mon 16:30 S052

The effect of surface oxidation on spin scattering for the W(110) surface — •Stephan Borek[1], Jürgen Braun[1], Jan Minár[1,2], Dima Kutnyakhov[3], Hans-Joachim Elmers[3], Gerd Schönhense[3], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universität München — [2]University of West Bohemia Pilsen — [3]Johannes-Gutenberg-Universität Mainz

It is well known that the W(110) surface possess interesting properties due to spin-orbit induced splitting of surface states. In our work we investigated the spin-orbit induced scattering of electrons from a clean W(110) surface using corresponding diffraction patterns to get an overview on the scattering behaviour. It was found that an oxygen passivation of the W(110) surface with a full oxygen overlayer has a huge impact on the electron diffraction. The oxidation of the W(110) surface reduces the spin-orbit asymmetry and the figure of merit whereas the reflectivity is increased. To investigate the surface electronic structure we calculated angle-resolved photoemission spectra using the fully-relativistic one-step model. Additionally, we will discuss the impact of full potential calculations on the spin-resolved diffraction patterns of spin-polarized electrons.

O 13.7 Mon 16:45 S052

Tuning magnetic coupling between organic-metal hybrids mediated by a nanoskyrmion lattice — •Maciej Bazarnik[1], Jens Brede[2], and Roland Wiesendanger[1] — [1]Dept. of Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany — [2]Donostia International Physics Center, Paseo Manuel de Lardizabal 4 20018 Donostia - San Sebastian, Spain

Molecular spintronic devices offer great potential for future energy-efficient information technology as they combine ultimately small size, high-speed operation, and low-power consumption. There are two approaches to molecular spintronics: first, to utilize the intrinsic properties of molecules by depositing them on weakly interacting surfaces like thin film insulators, graphene, or gold; second, to make use of new properties of organic-metal hybrids created by strong hybridization of molecular orbitals with the substrate such as iron films on iridium [1].

Here, we take the latter approach to control the magnetic properties of organic-metal hybrids and tune the magnetic coupling. We show how to position fullerene molecules on the skyrmionic lattice of a single atomic layer of iron on an iridium substrate utilizing the STM-based atomic manipulation techniques, in order to tune the magnetic interactions between them.

[1] J. Brede *et al.* Nature Nano. 9 (2014) 1018-1023

O 13.8 Mon 17:00 S052

Spin manipulation by creation of single-molecule radical cations — •Sujoy Karan[1,2], Na Li[3], Yajie Zhang[4], Yang He[3], I-Po Hong[3], Huanjun Song[4], Jing-Tao Lü[5], Yongfeng Wang[1,3], Lianmao Peng[3], Kai Wu[4], Georg S. Michelitsch[6], Reinhard J. Maurer[6], Katharina Diller[6], Karsten Reuter[6], Alexander Weismann[1], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93053 Regensburg, Germany — [3]Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, P. R. China — [4]College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P. R. China — [5]School of Physics, Huazhong University of Science and Technology, 1037 Luoyu Road, Wuhan 430074, P. R. China — [6]Lehrstuhl für Theoretische Chemie, Technische Universität München, 85747 Garching, Germany

All-trans-retinoic acid (ReA), a closed-shell organic molecule comprising only C, H, and O atoms, is investigated on a Au(111) substrate using scanning tunneling microscopy and spectroscopy. In dense arrays single ReA molecules are switched to a number of states, few of which carry a localized spin as evidenced by conductance spectroscopy in high magnetic fields. The spin of a single molecule may be reversibly switched on and off without affecting its neighbors. We suggest that ReA on Au is readily converted to a radical by the abstraction of an electron.

O 13.9 Mon 17:15 S052

Enantiomer-dependent spin orientation in photoelectron transmission through heptahelicene molecules — •Matthias Kettner[1], Johannes Seibel[2], Daniel Nürenberg[1], Karl-Heinz Ernst[2], and Helmut Zacharias[1] — [1]University of Münster, Center for Soft Nanoscience and Physikalisches Institut, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]EMPA, Nanoscale Materials Science, Überlandstrasse 129, 8600 Dübendorf, Switzerland

The interaction of electrons with helical molecules attains growing interest due to a spin selectivity in electron transmission. Experiments on self-assembled monolayers of double stranded DNA and oligopeptides [1] indicated a very efficient spin filtering behavior of the molecules at room temperature.

In present experiments enantiopure M- and P-heptahelicene molecules are evaporated onto different metal single crystal surfaces. The molecules arrange themselves to a highly ordered monolayer [2]. Samples are then irradiated with $\lambda = 213$nm laser radiation to generate photoelectrons from the substrate. These electrons are transmitted through the heptahelicene layer and analyzed with regard to their average longitudinal spin orientation by Mott scattering. The sign of the spin polarization depends on the helicity of the enantiomer. The effect of the heptahelicene on the spin orientation seems to be independent on the substrate.

References

[1] Kettner, M. et al., J.Phys.Chem. C 2014, 119, 26
[2] Seibel, J. et al., J.Phys.Chem. C 2014, 118, 29135

O 14: Surface Chemical Dynamics

Time: Monday 15:00–18:00 Location: S053

O 14.1 Mon 15:00 S053

The Importance of Meta-Stable Structures and High Spin States for Oxygen Activation on Small Gas-Phase Silver Clusters from First Principles — •Weiqi Wang, Luca M. Ghiringhelli, and Matthias Scheffler — *Fritz-Haber-Institut der MPG, Berlin.*

At finite temperature, the silver-cluster catalysts could have transient meta-stable structures with spin states higher than those of zero kelvin stable structures (singlets for an even number of silver atoms). These transient structures could be crucial in activating adsorbed species like O_2. In this work, the temperature-dependent relative stability of Ag_n and Ag_nO_2 ($n = 4, 8$) systems are simulated at different finite temperatures, by means of replica-exchange *ab initio* molecular dynamics (REMD) and efficient Boltzmann-reweighting based methods (e.g., Weighted Histogram Analysis Method, WHAM, and multistate Bennett acceptance ratio estimator, MBAR). The multi-spin-state free energy surfaces are visualised with the help of Sketch-Map [1]. The results show that meta-stable structures and the spin-polarized states can synergistically influence the activation of the adsorbed O_2 molecule. [1] M. Ceriotti, G. A. Tribello, M. Parrinello, J. Chem. Theory Comput. 9, 1521 (2013)

O 14.2 Mon 15:15 S053

Long-lived reactive trapped electrons on amorphous ice surfaces — •Sarah King[1], Daniel Wegkamp[1,2], Michael Meyer[1], Martin Wolf[1], and Julia Stähler[1] — [1]Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]ICFO - Institute of Photonic Sciences, Mediterranean Technology Park, Av. Carl Friedrich Gauss 3, 08860 Castelldefels (Barcelona), Spain

Trapped electron states have been observed for the first time at the amorphous solid water (ASW)/vacuum interface with relaxation times fourteen orders of magnitude longer than previously observed in bulk ASW. The formation, relaxation and decay pathways, and reactivity of trapped electrons was investigated using time-resolved two-photon photoemission of $\gtrsim$15 bilayers of D_2O on the Cu(111) surface. We find that the decay time of the trapped electron is 15.74 ± 0.12 s, independent of ASW thickness, suggesting an electron hopping mechanism, as opposed to tunneling, for electron recombination with the Cu surface. An increase in the ASW/Cu effective work function of approximately 0.5 eV, concomitant with a decrease in the photo-stationary trapped electron population, is also observed upon repeated irradiation of the ASW/Cu surface with ultraviolet femtosecond pulses. This is consistent with a reaction between the trapped electrons and the ASW at the vacuum interface producing an anionic species, and highlights the possible role of these trapped electrons as reactive intermediates.

O 14.3 Mon 15:30 S053

Reaction-diffusion modeling of hydrogen in beryllium — •Mirko Wensing, Dmitry Matveev, and Christian Linsmeier — Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany

Beryllium will be used as first-wall material for the future fusion reactor ITER as well as in the breeding blanket of DEMO. In both cases it is important to understand the mechanisms of hydrogen retention in beryllium. In earlier experiments with beryllium [1] low-energy binding states of hydrogen were observed by thermal desorption spectroscopy (TDS) which are not yet well understood. Two candidates for these states are considered: beryllium-hydride phases within the bulk and surface effects. The retention of deuterium in beryllium is studied by a reaction rate approach using a coupled reaction diffusion system (CRDS)-model relying on ab initio data from density functional theory calculations (DFT). In this contribution we try to assess the influence of surface recombination. [1] M. Reinelt, A. Allouche, M. Oberkofler, C. Linsmeier, New J. Phys. 11 043023 (2009)

O 14.4 Mon 15:45 S053

Deuterium/Wasserstoff-Isotopenaustausch an Beryllium und Berylliumnitrid — •Petra Dollase, Michael Eichler, Martin Köppen, Timo Dittmar und Christian Linsmeier — Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany

In den Fusionsexperimenten JET und ITER besteht die erste Wand im Hauptraum aus Beryllium (Be). Zur Strahlungskühlung im Divertor wird der Einsatz von Stickstoff diskutiert. Dieser kann mit der Oberfläche der ersten Wand zu Berylliumnitrid (Be_3N_2) reagieren. Als Brennstoff werden die Wasserstoffisotope Deuterium und Tritium eingesetzt, die in der Fusionsreaktion zu Helium und einem Neutron reagieren. Da der magnetische Einschluss des Plasmas nicht perfekt ist, treffen auch Deuterium- und Tritiumionen auf die Berylliumwand auf und können sich dort anreichern. Das soll aufgrund der Radioaktivität von Tritium unbedingt vermieden werden. Daher wird zur Regenerierung der ersten Wand der Isotopenaustausch mit Deuterium untersucht. Wir untersuchen den Isotopenaustausch von Deuterium und Protium, um nicht mit radioaktivem Tritium arbeiten zu müssen. Der Ionenbeschuss wird dabei mit einer Ionenquelle simuliert. Mit Spannungen bis maximal 5 kV werden Deuterium- und protische Wasserstoffionen in polykristallines Be bzw. Be_3N_2 implantiert. Die Proben werden dann in-situ mit Röntgenphotoelektronenspektroskopie (XPS) und thermischer Desorptionsspektroskopie (TDS) analysiert. Anschließend werden unter den gleichen Bedingungen hergestellte Proben ex-situ mittels nuklearer Reaktionsanalyse (NRA) charakterisiert.

O 14.5 Mon 16:00 S053

Untersuchung der Rückhaltemechanismen von Wasserstoff in Beryllium Wolfram Verbindungen — •Michael Eichler, Timo Dittmar und Christian Linsmeier — Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany

In den experimentellen Fusionsreaktoren JET und zukünftig auch ITER besteht die erste Wand im Hauptraum aus Beryllium (Be). In Bereichen der höchsten Wärmelasten (Divertor) wird zusätzlich Wolfram (W) verwendet. Als Brennstoff werden dieWasserstoffisotope Deuterium (D) und Tritium (T) eingesetzt. Durch den Kontakt der Reaktorwand mit den D- und T-Ionen wird unter anderem das Oberflächenmaterial erodiert und an anderen Stellen deponiert. Dadurch entstehen Be-W Verbindungen. Da das radioaktive T während des Reaktorbetriebs in der Wand eingelagert wird, ist die Untersuchung des Wasserstoffinventars, insbesondere der Rückhaltemechanismen in Be- W Legierungen von besonderem Interesse. Dazu wird das Ultra Hoch Vakuum Experiment namens ARTOSS vorgestellt, welches verschiedene Oberflächenanalytiken vereint und somit die in situ Präparation und Analyse entsprechender Materialien unter wohldefinierten Bedingungen ermöglicht. Der Ionenbeschuss im Reaktor wird hier mit einer Ionenquelle simuliert. Mit Spannungen bis maximal 20 kV werden Dund Wasserstoffionen in Be-W Verbindungen implantiert. Ausserdem werden erste Untersuchungen mittels Röntgenphotoelektronenspektroskopie (XPS), thermischer Desorptionsspektroskopie (TDS) und nuklearer Resonanzanalyse (NRA) gezeigt.

Invited Talk O 14.6 Mon 16:15 S053

In-situ Studies of the Reactivity of Pt Model Catalysts: from Flat Surfaces to Nanoparticles — •Christian Papp — Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg

Nanocluster arrays on supported graphene are intriguing model systems for catalysis, modeling the highly dispersed particles on real catalysts. We studied the adsorption and oxidation of CO and the chemistry of the catalyst poison SO_2 on Pt/Gr/Rh(111) with synchrotron-based high-resolution X-ray photoelectron spectroscopy.

On the Pt nanoclusters, we resolved CO adsorbed at three different sites, that is, on-top, bridge and step. The C 1s spectra exhibit remarkable similarities to those on single crystal surfaces: Similar to the case for stepped Pt(111) surfaces, a clear preference for the adsorption on the step sites is found, while the preference for the adsorption on the on-top site over the bridge site on the terraces is less pronounced than on Pt(111). Temperature-programmed X-ray photoelectron spectroscopy revealed an enhanced binding energy for the cluster step sites, similar to the situation on stepped Pt surfaces. The oxidation of CO follows roughly pseudo first order kinetics. The activation energy determined from an Arrhenius analysis was found to be smaller than for stepped and flat platinum crystals.

SO_2 adsorbs in two geometries, perpendicular and parallel to the surface, on both cluster facets and steps. While we again find a remarkable similarity to the adsorption situation on single crystals at low temperature, the reactivity of the nanoclusters is strongly increased.

Support by the DFG through SFB 953 is gratefully acknowledged.

O 14.7 Mon 16:45 S053

Temperature induced change in aliphatic monolayers observed by vibrational sum-frequency generation spectroscopy — •Andre Beier-Hannweg[1], Katharina Maus[1], Michael Lackner[1], Thorsten Balgar[2], Jan Weber[1], and Eckart Hasselbrink[1] — [1]Institut für Physikalische Chemie, Universität Duisburg-Essen — [2]Junior Uni-Wuppertal

The conformational order in long, aliphatic calcium-carboxylate Langmuir-Blodgett (LB) monolayers on solid glass supports is investigated by means of vibrational sum-frequency generation spectroscopy (VSFS). The C-H stretching vibrations of both the terminal methyl and the methylene groups are utilized to monitor the chain conformation at various sample temperatures. With increasing temperature, the LB-films exhibit structural changes, which can be probed by VSFS due to a difference in the corresponding signal-intensities at given temperatures. We will discuss how thermodynamic properties can be evaluated from the spectra.

O 14.8 Mon 17:00 S053

Reaction mechanisms by direct imaging of individual intermediates stabilized by surface dissipation and entropy — •Alexander Riss[1,2], Alejandro Pérez Paz[3], Sebastian Wickenburg[2,4], Hsin-Zon Tsai[2], Dimas G. de Oteyza[5,6], Angel Rubio[9,10,3], Felix R. Fischer[4,7,8], and Michael F. Crommie[2,4,8] — [1]Physik-Department E20, Technische Universität München, Germany — [2]Department of Physics, UC Berkeley, USA — [3]Nano-Bio Spectroscopy Group and ETSF, Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC & DIPC, San Sebastián, Spain — [4]Materials Sciences Division, LBNL, Berkeley, USA — [5]Donostia International Physics Center, San Sebastián, Spain and Ikerbasque, Basque Foundation for Science, Bilbao, Spain — [6]Centro de Física de Materiales CSIC/UPV-EHU-Materials Physics Center, San Sebastián, Spain — [7]Department of Chemistry, UC Berkeley, USA — [8]Kavli Energy NanoSciences Institute at the UC Berkeley and the LBNL, Berkeley, USA — [9]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [10]CFEL, Hamburg, Germany

We have directly determined the microscopic mechanisms underlying complex bimolecular coupling and cyclization reactions of enediynes through real-space imaging of the precise bond configuration of intermediate species using noncontact atomic force microscopy (nc-AFM). Supported by extensive theoretical calculations, we reveal that the observed transient intermediates along the reaction pathway are stabilized by efficient energy dissipation to the substrate and changes in molecular entropy along the reaction pathway.

O 14.9 Mon 17:15 S053

Exciting phonons: When molecules meet surfaces — •Vanessa Jane Bukas and Karsten Reuter — TU München, Germany

Exothermic surface chemical reactions may easily release several electron volts of energy. This challenges first-principles based dynamical simulations to account for adequate energy dissipation channels. Focusing on phononic dissipation, a novel embedding scheme for metallic substrates (QM/Me [1]) allows for energy to be dissipated out of a quantum-mechanically described reaction zone and into a computationally undemanding, yet reliably described, extended bath. In the application to oxygen dissociation over Pd(100) this approach predicted “hot” O adatoms traveling ballistically over several lattice constants as a consequence of non-immediate energy transfer to the surface [1].

Despite being similarly exothermic, a much shorter transient mobility was measured for the O_2/Pd(111) reaction [2]. We reconcile this apparent intricacy by quantitatively analyzing the underlying phonon excitations directly from QM/Me trajectories. This identifies certain groups of localized surface modes as the dominant dissipation channels, while comparing the Pd(100) and Pd(111) systems offers important trend understanding into the influence of surface symmetry. The thus obtained first-principles perspective on non-equilibrium adsorbate-phonon dynamics questions prevalent assumptions about energy sinks made in commonly used model Hamiltonians.

[1] J. Meyer and K. Reuter, Angew. Chem. Int. Ed. **53**, 4721 (2014).
[2] M.K. Rose *et al.*, Surf. Sci. **561**, 69 (2004).

O 14.10 Mon 17:30 S053

Inelastic Hydrogen Atom Scattering: Role of Electron-Hole Pair Excitations — •Oliver Bünermann, Hongyan Jiang, Yvonne Dorenkamp, and Alec Wodtke — Universität Göttingen, Institut für Physikalische Chemie, Tammannstr 6, 37077 Göttingen

Obtaining an atomic-level understanding of the dynamics of energy conversion at surfaces remains a complex and challenging area of modern research in physical chemistry. A general strategy to this field follows the lessons of gas-phase bimolecular chemical dynamics, where simple model systems are studied experimentally with great care while theoretical simulations are developed. One of the simplest systems to think of is Hydrogen atom scattering from a single crystalline surface. We built a new apparatus to experimentally investigate this model system with extraordinary precision. Laser photolysis is employed to produce a monochromatic H-atom beam. The H-atom beam strikes a single crystalline surface held in UHV. The kinetic energy and angular distributions of the scattered H-atoms are measured with extraordinary resolution employing Rydberg Atom Tagging.

Experimental results for scattering H-atoms from metal and insulator surfaces will be presented. In case of an insulator the scattering is nearly elastic while in case of metals strongly inelastic scattering is observed. Our results reveal that electron-hole-pair excitation is the dominate relaxation channel for H-atom translation in case of a metal surface, an interpretation supported by theoretical calculations [1].

[1] Buenermann, O et al., Science, DOI:10.1126/science.aad4972 (2015)

O 14.11 Mon 17:45 S053

Adatom Diffusion on Metal Surfaces: Disentangling Phononic and Electronic Energy Dissipation — •Simon P. Rittmeyer, Patrick Gütlein, and Karsten Reuter — TU München

The role of electron-hole pair excitations during dynamical surface processes on metal substrates has been controversially discussed. While adiabatic first-principles calculations often provide a satisfactory description, an abundance of such excitations is generally suggested by the continuum of electronic states around the Fermi level. With high-level non-adiabatic calculations still untractable for extended metal surfaces, the concept of electronic friction within the local density friction approximation (LDFA) offers numerically efficient, but approximate insight.

We have recently shown this approach to yield reasonable results for the vibrational damping of high-frequency adsorbate vibrations on various metal surfaces [1]. With this confidence we now apply it for surface diffusion, where non-adiabatic energy losses compete with energy losses due to phononic coupling. We compare our LDFA-based molecular dynamics simulations for various alkali-metal adsorbates on Cu(111) to experimental signatures obtained from ^{3}He spin echo measurements [2]. This comparison allows to decompose empirically obtained friction coefficients into electronic and phononic contributions for the first time.

[1] S.P. Rittmeyer *et al.*, Phys. Rev. Lett. **115**, 046102 (2015).
[2] D.J. Ward, PhD thesis, University of Cambridge (2013).

O 15: STM/AFM: New Approaches

Time: Monday 15:00–18:30 Location: H24

O 15.1 Mon 15:00 H24

Imaging Molecules in Atomic Force Microscopy with Carbon Monoxide Terminated Tips — •Nikolaj Moll, Leo Gross, Niko Pavliček, Bruno Schuler, and Gerhard Meyer — IBM Research – Zurich, Säumerstrasse 4, CH-8803 Rüschlikon, Switzerland

Using functionalized tips, the atomic resolution of a single organic molecule can be achieved by atomic force microscopy (AFM). We operate in the regime of short-ranged repulsive Pauli forces while the van-der-Waals and electrostatic interactions only add a diffuse attractive background. With atomic manipulation techniques we induce a on-surface transformation of an individual aromatic molecule into a highly strained 10-membered ring. The formation and breaking of the C–C bond is reversible which opens up the entire field of radical chemistry for on-surface reactions by atomic manipulation.

O 15.2 Mon 15:15 H24

Sub-molecular imaging by NC-AFM with an oxygen atom rigidly connected to a metallic probe — Oscar Díaz Arado[1], •Harry Mönig[1], Diego Rodríguez Hermoso[2], Milica Todorevic[2], Alexander Timmer[1], Simon Schüer[1], Gernot Langewisch[1], Rubén Pérez[2], and Harald Fuchs[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain

In scanning probe microscopy, the imaging characteristics in the various interaction channels crucially depend on the chemical termination of the probe tip. Here we analyze the contrast signatures of an O-terminated Cu tip with a tetrahedral configuration of the covalently bound terminal O atom. Supported by first-principles calculations, NC-AFM, and STM experiments, we show how this tip can be identified on a partially oxidized Cu(110) surface. After controlled tip functionalization, constant height NC-AFM imaging in the repulsive force regime reveals the internal bond structure of an organic molecule. In established tip functionalization approaches, the probe particles (e.g. CO or Xe) are only weakly bound to the metallic tip leading to lateral deflections during scanning. In contrast, our simulations for our tip show that lateral deflections of the terminating O atom are negligible. Its structural rigidity, chemically passivated state and a high electron density at the apex make the O-terminated Cu tip a highly attractive complementary probe for the characterization of organic nanostructures on surfaces.

O 15.3 Mon 15:30 H24

Influence of tip sharpness on subatomic resolution capability of atomic force microscopy — •Julian Berwanger, Ferdinand Huber, and Franz Josef Giessibl — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

By lateral manipulation, we show that the predicted diffusion barrier of 28.5meV of a single iron adatom [1] is lowered due to the presence of the tip by about 70% [2] and that the force responsible for manipulation is purely attractive for both Cu-terminated and CO-terminated tips. Moreover, we find that the metallic background of the functionalized tips strongly influences the tip-adatom interaction and the appearance of adatoms in the AFM channel. In a pyramidical tip model an increase of the apex angle from 126.0° to 126.9° already change the tip-adatom interaction from purely attractive to preferably repulsive. The tip with the apex angle of 126.0° can image adatoms at a by 30pm reduced tip-sample-distance compared to the tip with an apex angle of 126.9°. Subatomic resolution can only be obtained at relatively close tip-sample distances. Therefore we suggest that only "sharp" CO-terminated tips allow subatomic resolution [3]. [1] N. N. Negulyaev et al. PRB 79, 195411 (2009), [2] M. Emmrich et al. PRL 114, 146101 (2015), [3] M. Emmrich et al. Science 348, 308 (2015)

Invited Talk O 15.4 Mon 15:45 H24

Exploring chemical properties of surfaces by means of Atomic Force Microscopy — •Pavel Jelinek — Institute of Physics of the CAS, Cukrovarnicka 10, Praha, Czech Republic

Atomic resolution and manipulation is routinely achieved by both scanning tunneling microscopy (STM) and atomic force microscopy (AFM) nowadays. Despite of large activities in development of the technique, still some challenges remain, namely the chemical sensitivity on atomic level. It was demonstrated that AFM force spectroscopy could provide chemical identity of single atoms [1,2]. In this talk we present two novel methods extending further the chemical sensitivity of AFM. Electronegativity has been an important concept in chemistry, originally defined by Pauling as 'the power of an atom in a molecule to attract electrons to itself'. However its experimental determination is very limited. We present a new methodology to measure Pauling's electronegativity of individual atoms on surfaces by atomic force microscopy (AFM). Secondly we show that molecular recognition can be achieved using an analysis of characteristic minima (z_{min}(x,y) and df_{min}(x,y)) of 3D high-resolution maps combined with theoretical modeling.

[1] Y. Sugimoto et al Nature 446, 64 (2007) [2] M. Setvin et al ACS Nano 6, 6969 (2012)

O 15.5 Mon 16:15 H24

Atomic force microscopy reveals the structure of its tip and subatomic resolution on single iron adatoms — Matthias Emmrich[1], •Ferdinand Huber[1], Florian Pielmeier[1], Joachim Welker[1], Thomas Hofmann[1], Maximilian Schneiderbauer[1], Daniel Meuer[1], Svitlana Poleysa[2], Sergiy Mankovsky[2], Diemo Ködderitzsch[2], Hubert Ebert[2], and Franz J. Giessibl[1] — [1]Institute of Experimental and Applied Physics, Department of Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstraße 11, 81377 München, Germany

A CO molecule adsorbed on a Cu(111) surface can be used to probe the apex of an atomic force microscopy (AFM) tip [1]. In our recent work [2], we invert our previous experiment [1] and functionalize our tip with a CO molecule [3] to investigate single adatoms and clusters built from individual iron atoms adsorbed on a Cu(111) surface. Our findings correct our previous interpretation [1] and suggest that dual and triple minima in the force signal are caused by dimer and trimer tips, respectively [2]. However, we show subatomic resolution AFM: single iron adatoms do not appear as a single depression or protrusion, but as a toroidal structure. Its shape reflects the bonding symmetry of the adatom to the underlying substrate. Density functional theory (DFT) calculations support the experimental data.

[1] J. Welker and F. J. Giessibl, Science **336**, 444 (2012)
[2] M. Emmrich, F. Huber *et al.*, Science **348**, 308 (2015)
[3] L. Gross *et al.*, Science **325**, 1110 (2009)

O 15.6 Mon 16:30 H24

High-resolution AFM/STM imaging and force spectroscopy of van der Walls nanostructures on metal surface — •Martin Svec[1], Oleksander Stetsovych[1], Jan Berger[1], Pavel Hobza[2], and Pavel Jelinek[1] — [1]Institute of Physics AS CR, Prague, CZ — [2]Institute of Organic Chemistry and Biochemistry AS CR, Prague, CZ

Proper theoretical description of the weak vdW interaction, despite the large effort, still remains elusive and is intensely investigated. We prepared and investigated vdW nanostructures made of CO and Xe co-deposited on Ag(111) surface by a high-resolution 3D mapping with the AFM technique. We identify the atomic structure of such formations. In addition, we use the force-distance spectroscopy data, acquired with functionalized (CO, Xe) tips to gain direct access to the vdW forces acting between two well-defined systems. Such information provides a unique opportunity to benchmark the available theoretical methods employed to describe the vdW interaction. We will provide a direct comparison of various vdW methods to the experimental data.

O 15.7 Mon 16:45 H24

Intramolecular force contrast and dynamic current-distance measurements at room temperature — •Sonia Matencio[1,2], Ferdinand Huber[1], Alfred J. Weymouth[1], Carmen Ocal[2], Esther Barrena[2], and Franz J. Giessibl[1] — [1]Department of Physics, University of Regensburg, Germany — [2]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain

AFM can be used to probe the internal atomic structure of molecules [1]. Intramolecular resolution requires an unreactive tip and has been achieved at low temperatures. In the presented work we demonstrate intramolecular and intermolecular force contrast at room temperature on PTCDA molecules adsorbed on a Ag/Si(111)$-\sqrt{3}\times\sqrt{3}$ surface [2].

In addition, the oscillating force sensor allows us to dynamically measure the vertical decay constant of the tunneling current, κ [3]. The precision of the κ measurement was increased by quantifying the transimpedance of the current to voltage converter and accounting for the tip oscillation. The obtained κ maps show contrast between the two non equivalent PTCDA molecules of the herringbone phase giving evidence of a different tunneling barrier height.

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

[2] F. Huber, S. Matencio et al. Phys. Rev. Lett. 115, 066101 (2015).

[3] M. Herz et al. Appl. Phys. Lett. 86, 153101 (2005); G. Binnig et al. Surf. Sci. 126, 236 (1983).

O 15.8 Mon 17:00 H24

Sub-molecular resolution imaging of molecules by AFM: Pauli versus Coulomb — Joost van der Lit[1], •Nadine J. van der Heijden[1], Francesca Di Cicco[1], Prokop Hapala[2], Pavel Jelinek[2], and Ingmar Swart[1] — [1]Condensed Matter and Interfaces, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, The Netherlands — [2]Institute of Physics, Academy of Sciences, Prague, Czech Republic

In the past year, the origin of the contrast mechanism responsible for sub-molecular resolution imaging of molecules with functionalized tips has been a point of great discussion [1-3]. Especially the flexibility of the probe contributes to the high spatial resolution. Initially, van der Waals and Pauli interactions were thought to be responsible for the tip bending. Recently, it has been realized that also electrostatic forces influence the contrast [4]. Here, we study the role of the electrostatic force on the tip by imaging strongly polarized molecules with differently polarized tips. The charge on the final atom of the tip can be varied by different tip termination. CO tips yield nearly neutral tips while Xe terminated tips have a slight positive charge. This results in a difference in contrast in the final AFM image. References: [1] P. Hampala, PRB, 80, 085421, (2014). [2] J. Zhang, Science, 342, 611, (2013). [3] S. Hämäläinen, Phys. Rev. Lett. 113, 186102 (2014). [4] P. Hapala, Phys. Rev. Lett. 113, 226101 (2014).

O 15.9 Mon 17:15 H24

Extending carbon monoxide front atom identification (COFI) to probe the second atomic layer of an AFM tip — •Daniel Meuer, Andreas Bartholomäus Kelbel, and Franz Josef Giessibl — Universität Regensburg, Germany

The structural details of the tip determine the spatial resolution and the contrast which is obtained in atomic force microscopy. Welker and Giessibl demonstrated, that a CO molecule on a Cu(111) surface can characterize the foremost atomic layer of the apex of a metallic tip [1]. A detailed knowledge of the second atomic layer of the tip would allow even more insights into the tip structure.

In COFI, the upright bonded CO molecule on, e.g. Cu(111) probes the front atoms of the tip. We present a new technique where we put a CO on a Cu adatom essentially lengthening the CO molecule to a CuCO molecule. Then we trace the tip along a bell shaped curve to be closer to the second layer atoms next to the front most atoms. This method, which we call CuCOFI, allows us to characterize even the second atomic layer of the tip apex in situ by AFM.

References: [1] J. Welker and F. J. Giessibl, Science 336, 444 (2012)

O 15.10 Mon 17:30 H24

Understanding high-resolution AFM images of water clusters on NaCl substrate — •Prokop Hapala[1], Jing Guo[2], Jinbo Peng[2], Duanyun Cao[2], Limei Xu[2], Enge Wang[2], Ying Jiang[2], and Pavel Jelinek[1] — [1]Institute of Physics , Academy of Sciences of the Czech Republic, Cukrovarnická 10, Prague, 16253, Czech Republic — [2]International Center for Quantum Materials (ICQM) and School of Physics, Peking University, Beijing 100871, China

AFM using functionalized tips not only reveals chemical bonds within molecules [1], but it is also an ideal tool for sensing of non-covalent interactions. Recently we uncovered, using our molecular mechanics model [2], a crucial importance of electrostatic interaction in AFM images of various polar molecules [3]. In this talk we will show that the AFM imaging of water clusters formed on NaCl surface [4] is also governed by electrostatic field originating from both the polar O-H bonds and the ionic surface. The theoretical and experimental comparison between CO and Cl modified tip indicate that chiral pattern observed with negatively charged Cl tip is predominantly due to electrostatics. The ability to acquire and understand high-resolution AFM images of weakly bonded systems opens new possibilities of AFM in supramolecular chemistry and biochemistry. 1. Gross, L. et, al. Science 325, 1110-1114 (2009). 2. Hapala, P. et al. Phys. Rev. B 90, 085421 (2014). 3. Hapala, P. et al. (2015) (submitted) 4. Guo, J. et al. Nat. Mater. 13, 184-9 (2014).

O 15.11 Mon 17:45 H24

Scanning quantum dot microscopy made faster — •Christian Wagner[1,2], Michael Maiworm[3], Christian Müller[3], Matthew F. B. Green[1,2], Philipp Leinen[1,2], Eric Bullinger[3], Rolf Findeisen[3], F. Stefan Tautz[1,2], and Ruslan Temirov[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Institute for Automation Engineering (IFAT), Otto-von-Guericke University Magdeburg, Germany

Scanning quantum dot microscopy (SQDM) is a novel NC-AFM based scanning probe method that allows for the measurement of electric potentials with high sensitivity and spatial resolution[1]. To record SQDM images a single organic molecule is attached to the probe tip. This sensor molecule works as a quantum dot that can be charged via tunneling to or from the tip, depending on the local electrostatic potential. In a $\Delta f(V)$ spectrum the charging event causes a sharp dip, the position of which is the actual quantity of interest. The sharpness of this dip ($\approx$ 30 meV) suggests that methods beyond $\Delta f(V)$ spectroscopy could be used to measure its position, allowing image acquisition time to decrease from hours to minutes, making the method more versatile and easy to use. We discuss an approach to this task that is based on concepts from control theory such as system identification and extremum seeking controller.

[1] C. Wagner, M.F.B. Green, P. Leinen, T. Deilmann, P. Krüger, M. Rohlfing, R. Temirov, and F.S. Tautz, *Phys.Rev.Lett.* **115**, 026101 (2015).

O 15.12 Mon 18:00 H24

The energy resolution function of a tunnel junction — •Christian R. Ast[1], Berthold Jäck[1], Jacob Senkpiel[1], Matthias Eltschka[1], Markus Etzkorn[1], Joachim Ankerhold[2], and Klaus Kern[1,3] — [1]MPI für Festkörperforschung, 70569 Stuttgart — [2]Institut für Komplexe Quantensysteme and IQST, Universität Ulm, 89069 Ulm — [3]ICMP, EPFL, 1015 Lausanne, Switzerland

The tunnel junction between tip and sample in a scanning tunneling microscope is an ideal platform to access the local density of states in the sample through the differential conductance. We show that the energy resolution that can be obtained is principally limited by the electromagnetic interaction of the tunneling electrons with the surrounding environmental impedance as well as the capacitative noise of the junction. The parameter tuning the sensitivity to the environmental impedance is the capacitance of the tunnel junction. The higher the junction capacitance, the less sensitive the tunnel junction to the environment resulting in better energy resolution. Modeling this effect within P(E)-theory, the P(E)-function describes the probability for a tunneling electron to exchange energy with the environment and can be regarded as the resolution function of the tunnel junction. We experimentally demonstrate this effect in a scanning tunneling microscope with a superconducting aluminum tip and a superconducting aluminum sample at a base temperature of 15 mK, where it is most pronounced.

O 15.13 Mon 18:15 H24

Scanning Tunneling Microscopy at 20 mK — •Timofey Balashov, Michael Meyer, and Wulf Wulfhekel — Physikalisches Institut, KIT, Karlsruhe, Germany

We present a compact experimental setup for scanning tunneling microscopy and spectroscopy at 20 mK. To achieve this temperature, the microscope is mounted in a bath cryostat containing a ^{3}He/^{4}He dilution system. High mechanical stability and low electronic noise ensure a high energy resolution below 50 μeV. Additional capabilities include a 6 T axial magnetic field, quick tip and sample exchange and deposition of materials at low temperatures.

The high energy resolution enables precise measurements of complicated electronic systems and inelastic excitations. To demonstrate the capabilities of the instrument, we show measurements of magnetic excitations of Fe atoms on Pt(111).

O 16: Surface State Spectroscopy II

Time: Monday 15:00–18:00 Location: H4

O 16.1 Mon 15:00 H4

Unoccupied band structure of MgO/Ag(100) — •Rebecca Pöschel, Gianluca di Filippo, Andrej Classen, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander Universtität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Magnesium oxide films were prepared by evaporating magnesium on a well-defined Ag(100) single crystal kept at 440 K in $5 \cdot 10^{-7}$mbar oxygen. Films of different thicknesses between 1 ML to 20 ML were deposited on the crystal. The samples were studied by monochromatic angle-resolved two-photon photoelectron spectroscopy (photon energies 3.05 eV - 3.38 eV and 4.56 eV - 4.71 eV) and by angle-resolved vacuum ultra-violet photoelectron spectroscopy (photon energy 21.2 eV). Due to the negative electron affinity of MgO the conduction band minimum is observed near the low-energy cut-off and the valence band maximum near the high-energy cut-off within same UPS spectrum. We determined the evolution of the band gap with increasing film thickness and had a more detailed look at the dispersion of the conduction band minimum and the valence band maximum for a 5 ML and 20 ML thick film. For films up to 10 ML we found an unoccupied surface state with a binding energy of 1.24 eV relative to vacuum level which shows a free-electron-like dispersion.

O 16.2 Mon 15:15 H4

Interfaces of h-BN on Ag(111) and Ag/Cu(111) — •Martin Schwarz[1], Manuela Garnica[1], Daniele Stradi[2], Johannes V. Barth[1], and Willi Auwärter[1] — [1]Physik Department E20, Technische Universität München, James Franck Str. 1, 85748 Garching, Germany — [2]Department of Micro- and Nanotechnology, Center for Nanostructured Graphene, Technical University of Denmark, Denmark

Silver has attracted increasing interest as a substrate for heteroepitaxial layers, since the growth of a silicene layer on its (111) face has been demonstrated [1]. We explored different synthesis methods of hexagonal boron nitride (h-BN) layers on silver substrates. Beside the direct growth of h-BN on Ag(111), Ag intercalation on the BN/Cu(111) system [2] was investigated. The quality of the resulting layers has been examined by high-resolution scanning tunneling microscopy while the electronic structure of the Ag surface upon 2D layer growth has been studied by scanning tunneling spectroscopy and first-principle calculations. We demonstrate that the adsorption of the 2D layer alters the surface potential and has an impact on the binding energy of the Shockley-state which shifts towards higher energies.

[1] Lalmi, B. et. al. Appl. Phys. Lett., 2010, 97, 223109

[2] Joshi, S. et. al. Nano Lett., 2012, 12, 5821-5828

O 16.3 Mon 15:30 H4

A XPS/XPD study of the topological insulator BiTe — •Philipp Espeter[1,2], Sven Döring[2,3], Markus Eschbach[3], Matthias Gehlmann[2,3], Christoph Keutner[1,2], Christopher Kohlmann[1], Dominique Krull[1,2], Lukasz Plucinski[3], Ulf Berges[1,2], Claus M. Schneider[3], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4, D-44227 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund — [3]Forschungszentrum Jülich, D-52425 Jülich

Three-dimensional topological insulators are considered being a new state of quantum matter. They show an electronic bulk band structure with an insulating gap while they also possess metallic and highly spin-polarized surface states. Since the most interesting effects occur at the surface of topological insulators, a precise knowledge of the surface morphology and structure is crucial to understand its electronic structure.

In this study, we demonstrate a surface structure investigation of the weak topological insulator Bi_1Te_1 by means of photoelectron spectroscopy (XPS) and photoelectron diffraction (XPD). These measurements provide chemical as well as structural information of the sample surface.

The XPD pattern reveal that twelve different surface terminations are present on top of the sample. Furthermore, we monitored slight scaling effects and a shifting of individual Bi and Te layers.

O 16.4 Mon 15:45 H4

X-ray spectroscopic studies of the electronic structure of chromium based *p*-type transparent conducting oxides — •Emma Norton[1,2], Leo Farrell[1,2], Stephen Callaghan[1], Cormac McGuinness[1], Igor Shvets[1,2], and Karsten Fleischer[1,2] — [1]School of Physics, Trinity College, University of Dublin, Dublin 2, Ireland — [2]Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN)

The valence band structure of p-type transparent oxides - crystalline $Mg_xCr_{2-x}O_3$ and nanocrystalline Cu_xCrO_y- is analysed as a function of incoming photon energy. Comparisons with crystalline $CuCrO_2$:Mg are made, the best performing p-type transparent conducting oxide to date. The valence band of both p-type transparent conducting oxides show striking similarities to measurements on crystalline $CuCrO_2$ with all films showing that chromium states compose the top of the valence band, highlighting the important role of the Cr-O octahedra on the electronic structure.

O 16.5 Mon 16:00 H4

***In operando* strain-dependent HAXPES of VO_2 thin films on piezoelectric PMN-PT** — •Arndt Quer[1], Kerstin Hanff[1], Matthias Kallaene[1], Adrian Petraru[2], Lars-Philip Oloff[1], Hermann Kohlstedt[2], and Kai Rossnagel[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany — [2]Department of Nanoelectronics, University of Kiel, 24143 Kiel, Germany

The class of transition-metal oxides provides candidate materials for the realization of so-called Mottronic devices that make use of ultrafast and energy-efficient switching between distinct states of correlated electrons.

A paradigmatic material is VO_2, which undergoes a first-order structural transition from a low-temperature monoclinic phase to a high-temperature rutile phase at a transition temperature of about 340 K and simultaneously switches from insulating to metallic behavior by a five orders of magnitude resistance jump.

Interestingly in VO_2 films, insulator-to-metal transition can be tuned to some degree.

Here we use hard x-ray photoelectron spectroscopy (HAXPES) to directly study the electronic structure changes in VO_2 films on PMN-PT substrates as a function of temperature and in situ applied lattice strain.

Our results show clear changes in shape and position of the core level induced by strain and ferroelectric influence at the device-interface of the PMN-PT substrate.

O 16.6 Mon 16:15 H4

Rashba Spin-Orbit Coupling in the Presence of Ferroelectricity: Ultrathin Bi-films on BaTiO3 (001) — •Peter Lutz, Tim Figgemeier, Hendrik Bentmann, and Friedrich Reinert — Experimentelle Physik VII and Röntgen Research Center for Complex Materials (RCCM), Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The merging of two different material systems with specific physical properties provides a promising way to explore unique and new functunalities. In the case of ultrathin Bismuth (Bi) films on Barium Titanate (BTO) it was theoretically shown that the electric polarization of the ferroelectric substrate allows to manipulate the Rashba split Bi 6p states at the Fermi level [1]. By highly-ordered film growth we experimentally realized the formation of spin-orbit split surface states on ferroelectric BTO. The electronic structure looks similar to the one of pure Bi(111) or Bi/Si(111) but the films on BTO grow in thicknesses down to two bilayers [2]. This enables an enhanced coupling between the substrate and the Bi states. In our angle-resolved photoelectron spectroscopy (ARPES) data we investigated changes in the electronic structure of the electronic states when the ferroelectric substrate is driven through its structural phase transition [3]. Due to its capability of manipulating spin split states Bi/BTO may be regarded as a model system in realizing spintronic devices.

[1] H. Mirhosseini et al., Phys. Rev. B, 81, 073406, (2010) [2] T. Hirahara et al., Phys. Rev. Lett., 97, 146803 (2006) [3] W. Zhong et al., Phys. Rev. Lett., 73, 1861 (1994)

O 16.7 Mon 16:30 H4

Giant Circular Dichroism in Soft X-Ray Photoemission From Non-Magnetic Solids — •O. Fedchenko[1], K. Medjanik[2], S. Chernov[1], D. Kutnyakhov[1], B. Schönhense[3], M. Ellguth[1], A. Oelsner[4], S. Däster[5], Y. Acremann[5], J. Viefhaus[6], W. Wurth[6,7], T.R.F. Peixoto[8], P. Lutz[8], C.-H. Min[8], F. Reinert[8], J. Braun[9], J. Minár[9], H. Ebert[9], H.J. Elmers[1], and G. Schönhense[1] — [1]Uni-Mainz — [2]Max IV Lab, Lund, Sweden — [3]Imperial College London,UK — [4]Surface Concept GmbH, Mainz — [5]ETH Zürich, Switzerland — [6]DESY, Hamburg — [7]CFEL, Uni-Hamburg — [8]Uni-Würzburg — [9]TU-München

We report on the first measurements of circular dichroism in the angular distribution (CDAD) of photoelectrons from W(110) in the soft X-ray range. The experiment was performed at beamline P04 of PETRA III, providing circularly-polarized photons in a wide energy range from 260-2400eV [1]. The novel technique of ToF k-microscopy [2] is ideal for the study of dichroism. The CDAD asymmetry is surprisingly large and reaches almost 100% in some regions. It can thus be used as tool for circular polarimetry throughout the soft X-ray range. CDAD shows a pronounced dependence on photon energy and k-vector. It depends on matrix elements and relative phases of partial waves, has previously been shown using conventional electron spectrometers [3].

Funded by BMBF (05K13UM2, 05K13GU3)

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O 16.8 Mon 16:45 H4

Effects of orbital composition in a pair of spin-orbit-split surface bands at Tl/Ge(111) — •Ph. Eickholt[1], P. Krüger[2], S.D. Stolwijk[1], A.B. Schmidt[1], and M. Donath[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Institut für Festkörpertheorie, Universität Münster, Germany

Surface states of the Tl/Si(111)-(1×1) [1-3] and Tl/Ge(111)-(1×1) surfaces are strongly influenced by spin-orbit-interaction (SOI), leading to peculiar spin textures. Our setup for spin- and angle-resolved inverse photoemission allows us to study the unoccupied spin-orbit-split surface states within the whole Brillouin zone. In general, the surface electronic structures of both systems are very similar. In particular, surface states with comparable properties are found along $\overline{\Gamma}\,\overline{\mathrm{K}}$, independent of the substrate. Close to the $\overline{\mathrm{M}}$ point, however, the spin splitting between a pair of surface *states* at Tl/Ge(111)-(1×1) is considerably smaller than the splitting of the equivalent surface *resonances* at Tl/Si(111)-(1×1) – despite the fact that the former ones are more localized at the heavy Tl atoms. The difference in spin splitting is counter-intuitive since SOI in these systems is mainly due to the heavy Tl atoms and, in addition, Ge is heavier than Si. In this talk, we will show that a peculiar combination of SOI and hybridization [4] gives rise to the surprising differences observed in the experiment.

[1] S.D. Stolwijk *et al.*, Phys. Rev. Lett. **111**, 176402 (2013)
[2] S.D. Stolwijk *et al.*, Phys. Rev. B **90**, 161109(R) (2014)
[3] S.D. Stolwijk *et al.*, Phys. Rev. B **91**, 245420 (2015)
[4] S.N.P. Wissing *et al.*, Phys. Rev. B **91**, 201403(R) (2015)

O 16.9 Mon 17:00 H4

Many body effects on Cr(001) surfaces: An LDA+DMFT study — •Malte Schüler[1,2], Stefan Barthel[1,2], Michael Karolak[3], Matthias Bode[4], Alexander I. Poteryaev[5], Alexander I. Lichtenstein[6], Mikhail I. Katsnelson[7], Giorgio Sangiovanni[3], and Tim O. Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany — [3]Institut für Theoretische Physik, Universität Würzburg, Germany — [4]Lehrstuhl für Experimentelle Physik II, Universität Würzburg, Germany — [5]M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, Ekaterinburg, Russia — [6]Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany — [7]Radboud University of Nijmegen, Institute for Molecules and Materials, Nijmegen, The Netherlands

The electronic structure of the Cr(001) surface with its sharp resonance at the Fermi energy is the topic of many experimental and theoretical works. It is so far unclear and controversially debated whether the origin of this resonance is an orbital Kondo or an electron-phonon coupling effect. We have combined ab-initio density functional calculations with dynamical mean field simulations to calculate the orbitally resolved spectral function and show that they agree well to (I)PES data. We conclude that the combination of the realistic description of the electronic structure and the dynamic treatment of local Coulomb interaction is necessary to describe the complex many body effect in d_{z^2} and $d_{xz/yz}$ orbitals, which forms the low energy resonance.

O 16.10 Mon 17:15 H4

Electronic correlations in two-dimensional surface triangular lattices — •Florian Adler[1], Gang Li[2], Andrzej Fleszar[2], Felix Reis[1], Werner Hanke[2], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We have examined the electronic structure of two related adatom systems, namely the $\sqrt{3}\times\sqrt{3}$ reconstructions of Sn on SiC(0001) and the γ-phase of Pb on Si(111). In either case, the adatoms form a congeneric two-dimensional triangular lattice on their respective substrate, leaving one dangling bond unsaturated. Despite the half-filled surface band, both systems end up in a Mott insulating state due to electronic correlations. In order to grasp the emerging physics, we have analyzed their spectral functions using angle-resolved photoemission spectroscopy.

Interestingly, one clearly observes a qualitatively different distribution of spectral weight within the lower Hubbard band of the two systems. Depending on the strength of local and non-local Coulomb interactions as well as spin interactions, each system responds differently to the frustration imposed by the triangular geometry of the substrate. This results in a possible charge or spin order, which sets its fingerprint on the symmetry and weight distribution of the k-resolved spectral function. The responsible order mechanism can then be tracked down with the help of many-body calculations. First studies on the spectral functions and a comparison between the two systems will be presented.

O 16.11 Mon 17:30 H4

Interdependence of adsorption site and charge distribution in a single donor-acceptor molecule adsorbed on an ionic crystal — •Tobias Meier[1], Rémy Pawlak[1], Shigeki Kawai[1], Shi-Xia Liu[2], Yan Geng[2], Prokop Hapala[3], Pavel Jelínek[3], Alexis Baratoff[1], Silvio Decurtins[2], Ernst Meyer[1], and Thilo Glatzel[1] — [1]Department of Physics, University of Basel, Switzerland — [2]Department of Chemistry and Biochemistry, University of Bern, Switzerland — [3]Institute of Physics, Academy of Sciences of Czech Republic, Prague, Czech Republic

Electron donor-acceptor molecules are promising candidates for molecular electronic devices since they may generate separated electron-hole pairs upon absorption of photons or rectify electrical currents. Relevant properties of such complexes do not only depend on their intrinsic donor-acceptor character, but can also be modified by their interaction with the underlying surface. We used TTF-dppz [1], a fused pi-conjugated donor-acceptor molecule, deposited on insulating NaCl films on Cu(111). To investigate the interplay between the atomic structures of TTF-dppz and NaCl, we performed high-resolution STM and AFM measurements at 5 K. The charge distribution above individual molecules has been studied by local contact potential mapping [2,3]. We observed two different charge distributions which strongly depend on the adsorption site of the molecule. The results have been correlated with density functional theory calculations. [1] C. Jia et al., Chem. Eur. J. 13, 3804 (2007)., [2] S. Kawai et al., ACS Nano 7, 9098 (2013)., [3] B. Schuler et al., Nano Lett. 14, 3342 (2014).

O 16.12 Mon 17:45 H4

Two air- and water- stable ionic liquids in the presence of TaF5 and NbF5. Photoelectron Spectroscopy Study — •Anna Dimitrova[1], Marit Walle[1], Marcel Himmerlich[1], Stefan Krischok[1], Adriana Ispas[2], and Andreas Bund[2] — [1]Technische Universität Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, Deutschland — [2]Technische Universität Ilmenau, FG Elektrochemie und Galvanotechnik, Deutschland

Electroplating from Ionic Liquids has a great potential for deposition of metals and alloys with a Nernst potential below that of water decomposition. In order to control the electrochemical processes, an understanding of intra- and outer molecular interactions which take place before the metal electrochemical reduction is required. To this end we used Photoelectron Spectroscopy as a tool to study the electronic structure and the local environment of the atoms in thin films of a binary mixture - Ionic Liquids and TaF5 or NbF5. Two ionic liquids with a common anionic part were used: 1-butyl-1-methyl-pyrrolidinium bis(trifluoromethylsulfonyl)imide, [BMP][Tf2N] and 3-propyl-1-methyl-immidazolium bis(trifluoromethylsulfonyl)imide, [PMIm][Tf2N], in which TaF5 and NbF5 were separately dissolved in a different stoichiometry. In order to avoid the fast oxidation of both of the metal salts, the sample preparation and transportation to the Ultra-High Vacuum Chamber was done in an O2-free atmosphere. In this study the surface chemical compositions at different ionic liquid-to-metal salt concentration are discussed and compared with previous data, where ambient conditions were used for sample preparation.

O 17: Adsorption on Metal Surfaces

Time: Monday 15:00–18:15 Location: H6

O 17.1 Mon 15:00 H6

Self-assembly of Ni-TPP on the Cu (100) surface: electronic and geometric structure — •Giovanni Zamborlini[1], Vitaliy Feyer[1], Andrea Goldoni[3], Mirko Panighel[3], Giovanni Di Santo[3], Margherita Marsili[4,5], Paolo Umari[4], Bernd Kollmann[6], Daniel Lüftner[6], Peter Puschnig[6], and Claus M. Schneider[1,2] — [1]Peter Grünberg Institute (PGI-6), Research Center Jülich, 52425 Jülich, Germany — [2]Universität Duisburg-Essen, D-47048 Duisburg, Germany — [3]Elettra Sincrotrone Trieste, 34012 Basovizza, Trieste, Italy — [4]Dipartimento di Fisica e Astronomia, Università di Padova, 35141 Padova, Italy — [5]S3, Istituto Nanoscienze, CNR, 41125 Modena, Italy — [6]Institut für Physik, NAWI Graz, Karl-Franzens-Universität Graz, 8010 Graz, Austria

In this work the adsorption of the Ni-TPP on the Cu(100) surface was studied by a multi-technique approach combining STM, LEED and ARPES complemented by DFT. STM measurements show the presence of two rotational domains oriented with an angle of 16 degrees respect to each other, leading to a simulated superstructure which is in good agreement with the measured LEED pattern. Molecular orbital tomography was employed to determine the azimuthal orientation of the molecules as well as the molecule-substrate interaction and the charge transfer phenomena between adsorbed molecules and a metal surface. The valence band spectra of Ni-TPP/Cu(100) system show two features originating from the ionization of low energy molecular orbitals of adsorbed Ni-TPP. The experimental data are compared with DFT calculations.

O 17.2 Mon 15:15 H6

Is Cu$_2$N/Cu(100) a good insulator? An STM/STS study of a metal-organic monolayer — •Pascal R. Ewen[1,2], Cristian A. Strassert[2], Alexander A. Khajetoorians[2], and Daniel Wegner[2] — [1]Radboud Universteit, Nijmegen, The Netherlands — [2]Westfälische Wilhelms-Universtität, Münster, Germany

The study of molecules by scanning tunneling microscopy (STM) and spectroscopy (STS) also includes probing molecule-substrate interactions, which can change physical properties from hybridization to charge transfer and even to drastic effects such as decomposition. A thin insulating film can significantly decouple the adsorbate leading to a behaviour comparable to the isolated molecule. But it turns out that the decreased interaction with the substrate often causes drawbacks in the sample preparation or scanning conditions due to lower sticking coefficients or higher mobilities even at low temperature. In that respect, Cu$_2$N layers have recently gained increasing interest.

We investigate Pt(II) complexes that are used as emitters in prototypical OLEDs. Previously, we have shown that Pt-based orbitals are strongly influenced even by a Au(111) surface, which is commonly considered to show weak adsorbate-substrate interactions. Therefore, we have chosen to investigate the decoupling capability of Cu$_2$N/Cu(100) for these complexes. We found that the molecules self-assemble into a well-ordered monolayer. We determined adsorption geometry by STM and carefully analysed the spatial and energy distribution of molecular orbitals via STS-based spectral mapping to evaluate the impact of the substrate on the molecule.

O 17.3 Mon 15:30 H6

CO adsorption on graphene supported Pt, Rh and Pt-Rh nanoparticles — •Marcus Creutzburg[1,2], Heshmat Noei[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchroton (DESY), Notkestraße 85, Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, Jungiusstraße 9, Hamburg, Germany

Small metal nanoparticles dispersed on porous substrates have gained increasing interest in surface science because of their widespread applications, especially in heterogeneous catalysis. It was previously shown that nanoparticles grown by UHV vapor deposition of material form ordered arrays on graphene substrates using the moiré of graphene/Ir(111) as a template. The size and shape of these nanoparticles can be carefully controlled with diameters smaller than 2 nm on graphene/Ir(111) by the amount of deposited material. In this contribution, we study the adsorption of CO on Pt, Rh and Pt-Rh core-shell nanoparticles on graphene/Ir(111) using vibrational spectroscopy under UHV conditions. The UHV-IRRAS data demonstrate one adsorption site for the two-layered Pt and Rh nanoparticles, which is assigned to CO on-top edge sites of the nanoparticles, while for the three-layered Pt and Rh nanoparticles the adsorption of CO on-top edge sites is only preferred at low CO coverages. For higher CO coverages a second (additional) adsorption site with higher wavenumbers is observed, which is interpreted as on-top adsorption sites on nanoparticle terrace atoms. Three-layered Pt-Rh core-shell nanoparticles show CO adsorption on-top of Rh edge and corner atoms at low CO coverages and on-top of Pt terrace sites at higher CO coverages.

O 17.4 Mon 15:45 H6

STM study of tower-shaped tripodal molecules on a Au(111) surface — •Timo Frauhammer[1], Lukas Gerhard[1], Kevin Edelmann[1,3], Maximilian Kristen[1], Marcin Lindner[1], Michal Valasek[1], Marcel Mayor[1,2], and Wulf Wulfhekel[1,3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT) — [2]Department of Chemistry, University of Basel — [3]Physikalisches Institut, Karlsruhe Institute of Technology

We examined three different tetraphenylmethane derivates deposited on a Au(111) surface using scanning tunneling microscopy (STM) at 5 K. The molecules are designed as tripodal tower-shaped molecules with a platform that specifically binds to the Au surface and molecular rods of one to three phenyl rings pointing away from the surface with a nitrile end group to allow contact formation to the STM tip. We deposited the molecules from a solution with Dichloromethane by using a spray technique.

It is shown that up to a height of at least three phenyl-rings the molecules indeed stand upright on their tripodal sulfur-feet with the head group arranged away from the surface. For the three investigated molecules, the apparent height, the shape in constant current images and the conductance at constant height are compared.

O 17.5 Mon 16:00 H6

Line shapes of C$_{60}$ vibrational modes in inelastic electron tunnelling spectroscopy — •Stefan Meierott, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

Tunnelling contacts comprising W tips coated with Pb and terminated by single C$_{60}$ molecules as well as pristine and C$_{60}$-covered Pb(111) surfaces were investigated with a low-temperature scanning tunnelling microscope. The junctions exhibited C$_{60}$ vibrational signatures, which were previously observed [1]. While Pb-coated W tips led to peak-like line shapes of the vibrational modes in inelastic tunnelling spectra [1] C$_{60}$-terminated tips gave rise to Fano-type profiles. In agreement with previous calculations [2] we assign the Fano-type line shape to the electronic structure of the C$_{60}$-terminated tip. The lowest unoccupied molecular orbital (LUMO) of C$_{60}$ at the tip apex covered the range of vibrational energies, which was identified as a prerequisite for observing Fano-type line shapes [2]. To test the proposed scenario, the LUMO energy of C$_{60}$ attached to the tip was deliberately modified, presumably owing to different adsorption geometries at the tip apex [3]. Upon moving the LUMO energy farther away from the Fermi level and concomitantly avoiding its overlap with vibrational energies, the peak-like structures in the vibrational spectra were recovered. Financial support by the DFG through KR 2912/7-1 is acknowledged.

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[2] A. Baratoff et al., J. Vac. Sci. Technol. A **6**, 331 (1988).
[3] G. Schull et al., New J. Phys. **10**, 065012 (2008).

O 17.6 Mon 16:15 H6

Controlled Intermolecular Coupling in Charging Processes of Molecular Assemblies — •Nemanja Kocić[1], Dominik Blank[1], Silvio Decurtins[2], Shi-Xia Liu[2], and Jascha Repp[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Department of Chemistry and Biochemistry, University of Bern, 3012 Bern, Switzerland

In a recent study, we found that electron-acceptor molecules located at the edges of the self-assembled islands on the Ag(111) surface can be switched in their charge state by means of the electrostatic field inside a scanning tunneling microscope junction [1]. Here, we show that controlled vacancy formation by means of STM-based manipulation techniques allows to convert molecules inside the islands to edge-like molecules and thereby to create different pattern of molecules that show charge switching. Whereas simple electrostatic effects lead to different switching fields for different arrangements, in addition, very complex charging pattern originate from strong coupling between charge states of the molecules. Thereby, our work demonstrates that very complex functionality can be encoded into only few interacting molecules and might be a first step towards molecule-based cellular automata.

[1] N. Kocić et al., Nano Lett. 15, 4406 (2015)

O 17.7 Mon 16:30 H6

Reversible light-induced spin-state switching in Fe(II) spin-crossover films on Au(111) studied with NEXAFS and PES — •Sebastian Rohlf[1], Matthias Kalläne[1], Arndt Quer[1], Holger Naggert[2], Felix Tuczek[2], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany — [2]Institut für Anorganische Chemie, Universität Kiel, 24098 Kiel, Germany

Fe(II) coordination complexes are model systems for organic molecules whose electronic, magnetic, and structural properties can be manipulated by external stimuli. Moreover, the temperature- and irradiation-dependent spin transitions observed in a number of these materials may provide a suitable testbed for the development of future spintronic devices. Light-induced spin-state trapping (LIESST) in thin molecular films of these complexes is well established. Here, we present a combined near edge X-ray absorption fine structure (NEXAFS) and photoelectron spectroscopy (PES) study of the LIESST and, for the first time, of the reverse LIESST of thin films of the spin-crossover complex $Fe(H_2bpz)_2(phen)$ adsorbed on Au(111). The NEXAFS spectra reveal two different stable molecular spin states after green and infrared light irradiation at low temperatures. The PES results confirm these observations and, furthermore, provide information on the efficiencies of the light-induced transition processes.

O 17.8 Mon 16:45 H6

The interaction of deuterium with AgPd/Pd(111) surface alloys — •Thomas Diemant, Jan Martin, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Albert-Einstein-Allee 47, Ulm University, D-89081 Ulm

AgPd/Pd(111) surface alloys, which consist of a reactive and an inert metal, represent an ideal test case for the study of ensemble effects on bimetallic surfaces. In the present contribution, we have studied their deuterium adsorption properties by temperature-programmed desorption (TPD) measurements. The structural properties (surface contents and atom distribution) were determined already earlier by high-resolution scanning tunnelling microscopy (STM) [1], which enables us to correlate the structural properties of these surface alloys to their adsorption behaviour. Most prominently, a steady decrease of the adsorbate coverage with increasing Ag content is observed. The results will be compared to findings on the interaction of CO with these surface alloys [2].

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O 17.9 Mon 17:00 H6

Water - Hydroxyl Overlayers on Rh(111) — •Christine McMahon, Alan Masey, Andrew Hodgson, and George Darling — Surface Science Research Centre University of Liverpool Liverpool L69 3BX

At metal surfaces, water ice structures are determined by a competition between optimising the bonding of molecules to the surface and optimising the hydrogen bonding within the layer. On some metals the water overlayer is partially dissociated, this can be induced by preadsorbing oxygen, leading to a mixed OH+H2O overlayer on metals where dissociation is not spontaneous. We have used Density Functional Theory calculations to examine partially dissociated overlayers produced on Rh(111). Specifically we are looking to address questions that cannot be definitively answered by experiment: what is the optimum ratio of OH to H2O, and do the resultant structures favour Bjerrum defects (defects where H atoms point to each other rather than participating in hydrogen bonding or pointing into/away from the surface), as found on Cu surfaces.

O 17.10 Mon 17:15 H6

Adsorption of isolated nickelocene on Cu(100) — •Marisa Faraggi[1], Nicolas Bachelier[2], Maider Ormaza[2], Benjamin Verlhac[2], Martin Verot[3], Tangui Le Bahers[3], Marie Laure Bocquet[1], and Laurent Limot[2] — [1]Ecole Normale Supérieure, Département de Chimie, ENS-CNRS-UPMC UMR 8640, 75005 Paris, France — [2]IPCMS, Universite de Strasbourg, UMR CNRS 7504, 67034 Strasbourg, France — [3]Universite de Lyon, Universite Claude Bernard Lyon 1, CNRS, ENS Lyon, 69007 Lyon, France

In this work we focus on the study of nickelocene in gas phase and deposited on Cu(100). We concentrated on the theoretical description of the system by implementing Density Functional Theory (DFT) using the VASP code. We performed an energetic analysis of the adsorption of nickelocene in three high-symmetric sites by centering the Cp ring in a top, bridge and hollow site of Cu(100). We move within different theoretical approximations (PBE, Grimme, optPBE) to better describe the main characteristics of the system. Our results show that the hollow site appears to be energetically more stable in all approaches, in agreement with the STM experiments. Nickelocene is moderately chemisorbed. The atomic-orbital projected density of states were also studied. The lowest unoccupied molecular orbital (LUMO) of Nc is clearly spin polarized, giving a magnetic character to the molecule. Hence, the entire Nc molecule is magnetic and the magnetization is shared by the two Cp rings and by the dyz, dxz shells of the Ni atom. Upon adsorption the magnetic moment of nickelocene is therefore preserved.

O 17.11 Mon 17:30 H6

Chemo-mechanical coupling from first principles: On the strain dependency of oxygen adsorption on Pd(111) — •Gregor Feldbauer, Anja Michl, and Stefan Müller — Hamburg University of Technology, Institute of Advanced Ceramics, Denickestr. 15, D-21073 Hamburg

Mechanical deformation can affect the adsorption and reaction processes of reactants on surfaces. Thus, by straining catalytically active surfaces their reactivity as well as selectivity can be influenced, which is of high importance in the field of heterogeneous catalysis.

Here, the adsorption of atomic oxygen on Pd(111) is used as a model system. At first, the dependence of the adsorption energetics on various oxygen adsorption sites and coverages is investigated within the framework of density functional theory (DFT). Furthermore, vibrational frequencies, work functions and densities of states are studied. Using the DFT results as input data a cluster-expansion Hamiltonian is constructed to scan exhaustively the configuration space of the examined model system. This allows to identify the most favourable adsorption configurations. Additionally, for various configurations biaxial strain is applied in the surface plane to obtain the response of the adsorption energetics. Particularly, the coupling parameter between the strain and adsorption energies is of interest to allow for a comparison with experiments.

O 17.12 Mon 17:45 H6

Methanol oxidation on nanoporous gold — •Wilke Dononelli[1], Lyudmila Moskaleva[2], and Thorsten Klüner[1] — [1]IfC, CvO Universität Oldenburg, 26111 Oldenburg — [2]IAPC, Universität Bremen, 28359 Bremen

Nanoporous metals, such as nanoporous gold (np-Au), have recently attracted considerable interest due to their potential use in catalysis. These Au-based catalysts can be used for fuel cells, the synthesis of esters or the selective oxidation of alcohols, where the selectivity of gold to partial oxidation products is higher than the selectivity of other metal catalysts. For this study, a kinked Au(321) surface first introduced by Moskaleva [1] respresents one of the surfaces of the nanoporous gold. It consists of (111) terraces and zigzag-shaped steps, which may be favorable as possible adsorption positions for methanol in partial oxidation reactions. These catalytic surface reactions are analyzed using the exchange-correlation functional PBE and rPBE-D3 implemented in the plane-wave based Vienna ab initio simulation package (VASP) within the supercell approach. The aim is the elucidation of the detailed mechanisms for total and partial oxidation of methanol on this model surface. We will calculate the adsorption geometries for the reaction intermediates and transition states in order to identify the energetically most favorable reaction paths. Beyond that the effect of adsorbed active oxygen species like atomic oxygen, molecular oxygen or hydroxo and hydroperoxo species on the reaction mechanisms will be considered. [1] L.V. Moskaleva, V. Zielasek, T. Klüner, K.M. Neyman, M. Bäumer, Chem. Phys. Lett. 525 (2012) 87.

O 17.13 Mon 18:00 H6

A quantum chemical study of adsorption and catalytic activity on nanoporous gold (np-Au) surfaces — •Gabriele

Tomaschun[1], Lyudmila Moskaleva[2], and Thorsten Klüner[1] — [1]IfC, CvO Universität Oldenburg, 26111 Oldenburg — [2]IAPC, Universität Bremen, 28359 Bremen

The Nanotechnology is one of the most important future technology fields. The fact, that nanoparticles show an extraordinary relation between size and the properties of the material, allows us to use them in a variety of catalytic applications. The np Au as an example shows a remarkable catalytic activity even though bulk gold is catalytically inert. The reason for this is the high specific surface area and a high density of low coordinated surface atoms in the np Au surface. Various theoretical studies of the Au(111) and Au(321) [1] surfaces could well represent the catalytic behavior of the np Au ligaments. The Au(310) surface with steps, kinks and sinks in the terraces is an additional surface which has a lot of adsorption sites and thus can also very well describe the np Au surface. We represent the theoretical study of the methanol oxidation on the Au(310) model-surface with the purpose to find the feasible adsorption sites for different adsorbates and the favorable reaction pathways. In this study, we use the plane-wave based Vienna ab initio simulation package (VASP) [2] with the exchange-correlation functional PBE [3]. [1] L.V. Moskaleva, V. Zielasek, T. Klüner, K. M. Neyman, M. Bäumer, Chem. Phys. Lett. 525 (2012) 87. [2] G. Kresse, J. Hafner, Phys. Rev. B 49 (1994) 14251. [3] J. P. Perdew, K. Burke, M. Erzenhof, Phys. Rev. Lett. 77 (1996) 3865.

O 18: Metallic Nanowires on Semiconductor Surfaces

Time: Monday 17:00–19:30 Location: Poster A

O 18.1 Mon 17:00 Poster A

Stepped Silicon Surfaces: Exploring the Formation of Spin Chains — Julian Aulbach[1], •Tim Wagner[1], Steven C. Erwin[2], Ralph Claessen[1], and Joerg Schaefer[1] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, Germany — [2]Naval Research Laboratory, Washington DC, USA

Adsorption of a submonolayer of gold on various stepped Si(hhk) substrates yield the formation of atomic wire arrays with rather perfect structural order. As a specific representative, stabilization of the Si(553) surface by Au adsorption results in two different atomically defined chain types, one made of Au atoms and one of Si. The latter, situated at the step edges, forms a honeycomb nanoribbon which is subject to antiferromagnetic spin ordering [1, 2]. However, the extent to which the magnetic pattern can be modified, or suppressed, has remained unexplored. Here our approach is to exploit the tunability offered by the Si(hhk)-Au family, which exhibits not only varied terrace widths but also different bonding networks. Based on scanning tunneling microscopy and density-functional theory we reveal why magnetic patterns form on particular Si(hhk) surfaces but not on others, and propose broad strategies for using surface chemistry to control the formation or suppression of spin chains more generally.

[1] J. Aulbach et al., Phys. Rev. Lett. 111, 137203 (2013).
[2] S. C. Erwin and F. J. Himpsel, Nat. Commun. 1, 58 (2010).

O 18.2 Mon 17:00 Poster A

Observation of correlated spin-orbit order in a strongly anisotropic quantum wire system — •Monika Jäger, Christian Brand, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

Vicinal Si(557) surfaces covered by 1.31 ML Pb reveal a 1D transport behavior below 78 K [1]. The delicate interplay between the superlattice structure, band filling, and extremely large spin-orbit interaction results in a highly correlated entangled spin- and charge-state. Recent spin resolved ARPES measurements have shown that the insulating behavior across the direction of the wires is associated with the formation of a spin-orbit density wave [2, 3].

In order to correlate these findings with the morphology the atomic structure was investigated by means of STM. Adsorption of Pb at 600 K gives rise to a refacetting of the Si surface into a local (223) orientation with an average spacing of 1.58 nm. High resolution STM images have clearly identified $\sqrt{3} \times \sqrt{3}$ reconstructions on the $4\frac{2}{3} \times 0.332$ nm wide (111) terraces. The 0.665 nm periodicity along the terraces is superimposed by an additional intensity modulation which is compatible with a 10-fold periodicity deduced from the spot-splitting seen in former high resolution LEED measurements.

[1] C. Tegenkamp et.al. PRL **95**, 176804 (2005).
[2] C. Brand et.al. Nat. Comm. **6**, 8118 (2015).
[3] C. Tegenkamp et.al. PRL **109**, 266401 (2012).

O 18.3 Mon 17:00 Poster A

Structural and electronic instabilities in Si(hhk)-Au — •Marvin Detert, Timo Lichtenstein, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover

For future plasmonic devices understanding at low dimensional collective excitations is indispensable. For quasi one dimensional (1d) structures, Au induced wires on regularly stepped Si(hhk) offer the perfect playground. Therefore, Si(553) and Si(775) were prepared at coverages where both surfaces host a double atomic gold chain per terrace. All measurements were performed at a base pressure of 5×10^{-11} mbar by an electron energy loss spectrometer combined with a setup of spot profil analysis in low energy electron diffraction providing both high momentum and energy resolution.

As long time measurements showed a time dependent shift of the plasmon dispersion for Si(hhk)-Au at various Au coverages, the plasmonic excitations in Si(775)-Au and Si(553)-Au, particularly the dispersion relation and its time dependence, were investigated. Primarily we took special care to eliminate water and hydrogen from the background gas. We found that the plasmon dispersion remains unchanged over time for a coverage of 0.48 ML for Si(553)-Au and a coverage of 0.32 ML for Si(775)-Au. Therefore, at these coverages all dangling bonds seem to be saturated. At other coverages, thermal desorption spectroscopy shows mainly an H_2 peak at 580 °C. Therefore, we conclude that atomic hydrogen generated by the electron beam leads to a modification of structural and electronic properties.

O 18.4 Mon 17:00 Poster A

Local defects in quasi-1D Si(553)-Au — •Zamin Mamiyev, Timo Lichtenstein, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

Self-assembled quasi-1D metallic structures formed on vicinal Si surfaces are highly attractive due to their individual electronic states that are confined to a single spatial dimension. In this respect, metallic nanowires induced by Au atoms at the regularly stepped Si(553) surface exhibit a variety of interesting electronic properties which are determined by the atomic structure. In order to obtain a quantitative description of the chemically adsorbed residual gas (CO, H_2O, H_2) effect to plasmon loss, time dependent electron energy loss spectra were measured along the momentum transfer parallel ($q_{||}$) and perpendicular ($q_{\perp}$) to wires. Plasmon loss energy shows a linear decay of the adsorption probability as a function of active site concentration, and an exponential saturation of the additional coverage with time.

On the Si(553)-Au surface Au atoms are arranged in dimerized double chains per terrace and show a strong tendency to suffer structural transitions. Since the whole terrace is chemically active on the Si(553)-Au surface, it is conceivable that an adsorption of the additional atoms takes place on these chains. Due to strong chemical bonds, atomic hydrogen locally converts the Au chains into an insulator. Therefore, the atomic hydrogen adsorbed on the surface is limiting the propagation of collective modes.

O 18.5 Mon 17:00 Poster A

Au/Si(553) and Au/Si(111) surface phonons and Raman scattering efficiencies calculated from first principles — •Sergej Neufeld, Simone Sanna, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn

Metallic nanowires on semiconducting substrates have been attracting considerable interest in the last decades. Self organizing gold chains at vicinal surfaces such as the Si(553) and Si(111) are of particular interest, as the use of stepped templates allows to vary the geometric parameters and, thus, tune the inter-chain coupling. While microscopic structural models of Au nanowires on various Si surfaces are available in the literature, little is known about their vibrational properties in terms of surface localized phonon mode frequencies, eigenmodes and Raman scattering efficiencies. In this work, the phonon mode characteristics of the Au/Si(553) and Au/Si(111) surfaces are calculated from first-principles. Several surface localized phonon modes are found, whose phonon frequencies can be directly compared with the spectra obtained by Raman measurements. Additionally, the differential Raman cross section of the Au/Si(111) surface is calculated via linear response routines. A qualitative agreement between theoretical and experimental spectra could be observed.

O 18.6 Mon 17:00 Poster A

Au nanowires at Si(775): Structure, electronic bands and magnetic ordering calculated from first principles — •Christian Braun, Simone Sanna, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany

In recent years, one-dimensional systems have increasingly come into focus due to their interesting electronic properties including, inter alia, Peierls instabilities and Luttinger liquid behavior. Promising realizations of quasi-one-dimensional systems are, among others, self-assembled gold nanowires on vicinal Si(111) surfaces.

However, the exact structure of many gold deposited vicinal Si(111) surfaces are still unclear. In this work, various structures of gold chains on the Si(775) surface have been investigated by first-principles and, depending on the gold coverage, different models for this particular surface are proposed. These are supported by STM simulations and calculations of the band structure. Interestingly, we find the energetically most favored models to show a magnetic ordering, similar to the case of Au/Si(553) surface [1].

[1] SC Erwin, FJ Himpsel, Nature Commun. 1, 1 (2010).

O 18.7 Mon 17:00 Poster A

SPA-LEED investigations of quasi one dimensional Dysprosiumsilicide structures on Si(001) — •Jascha Bahlmann, Frederic Timmer, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

The investigation of rare earth metal induced nanowires on silicon is of particular interest due to their quasi one dimensional structure and the consequential electronic properties. Dy was deposited on flash-annealed Si(001) samples by means of physical vapor deposition (PVD) and examined by spot profile analysis low energy electron diffraction (SPA-LEED) as a function of the Dy coverage and the sample temperature.

(2 × 4)- and (2 × 7)-reconstructions are observed at lower coverages. The formation of these structures appears to be temperature-dependent. A bundling of the nanowires can be observed at sample temperatures of 500° C and higher coverages. In addition mean domain sizes were determined in order to derive the optimal growth parameters for the nanowires.

O 18.8 Mon 17:00 Poster A

Structural and electronic properties of rare-earth silicide thin films at Si(111) — •Christof Dues, Wolf Gero Schmidt, and Simone Sanna — Lehrstuhl für Theoretische Physik, Universität Paderborn, D-33095 Paderborn

Rare-earth (RE) silicides thin films on silicon surfaces are currently of high interest. They grow nearly defect-free because of the small lattice mismatch, and exhibit very low Schottky-barriers on n-type silicon. They even give rise to the self-organized formation of RE silicide nanowires on the Si(001) and vicinal surfaces.

Depending on the amount of deposited RE atoms, a plethora of reconstructions are observed for the RE silicide. While one monolayer leads to the formation of a 1×1-reconstruction, several monolayer thick silicides crystallize in a $\sqrt{3}\times\sqrt{3}$ R30° superstructure. Submonolayer RE deposition leads to different periodicities.

In this work we investigate the formation of RE silicides thin films on Si(111) within the density functional theory. The energetically favored adsorption site for RE adatoms is determined calculating the potential energy surface. As prototypical RE, Dysprosium is used. Additional calculations are performed for silicides formed by different RE elements. We calculate structural properties, electronic band structures and compare measured and simulated STM images. We consider different terminations for the 5 × 2 reconstruction occurring in the submonolayer regime and investigate their stability by means of *ab initio* thermodynamics. The same method is employed to predict the stable silicide structure as a function of the deposited RE atoms.

O 18.9 Mon 17:00 Poster A

Raman spectroscopy of quasi-1D nanowires on the Si(553)-Au surface — •Julian Plaickner[1], Sandhya Chandola[1], Eugen Speiser[1], Norbert Esser[1], Benedikt Halbig[2], Jean Guerts[2], Julian Aulbach[3], Jörg Schäfer[3], Sergej Neufeld[4], and Simone Sanna[4] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Berlin — [2]Universität Würzburg, Experimentelle Physik III, Würzburg — [3]Universität Würzburg, Experimentelle Physik IV, Würzburg — [4]Fakultät für Naturwissenschaften, Department Physik, Universität Paderborn

Vicinal Si(111) substrates offer an additional control parameter (terrace width) for growth of atomic gold chains on Si(111) terraces. Moreover, a new one-dimensional so-called Si honeycomb-like structure is generated, the latter exhibiting spin polarization effects at low temperature, according to calculations [1], accompanied by small structural changes at the step edges. Optical methods such as Reflectance Anisotropy Spectroscopy (RAS) and Raman spectroscopy have been shown to be sensitive tools to verify surface structure of such nanostructures. Here we concentrate on a study of the surface phonon modes of the Si(553)-Au-(5x2) surface by Surface Raman Spectroscopy.

Raman spectra Si(553)-Au-(5x2) surface show clear signatures of Au- and Si related surface vibrations, while RAS shows signatures of electronic surface transitions [2]. Additionally, the measurement of Raman spectra for different polarization configurations allows investigating the symmetry of the phonon modes. The comparison of Raman spectra taken at room temperature and low temperatures shows clear differences that can be related to specific structural elements of the surface. This suggests that a structural transition occurred between the two temperatures.

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. 1, 58 (2010)
[2] C. Hogan et al. PRL 111, 8, 087401 (2013)

O 18.10 Mon 17:00 Poster A

Optical properties and electronic doping of quasi-1D gold nanowires on vicinal Si surfaces — •Sandhya Chandola[1], Eugen Speiser[1], Julian Plaickner[1], Conor Hogan[2], Julian Aulbach[3], Jörg Schäfer[3], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Institute for Structure of Matter, National Research Council (CNR-ISM) Via Fosso del Cavaliere, 00133 Rome, Italy — [3]Universität Würzburg, Experimentelle Physik IV, Würzburg

The atomic structures of sub-monolayers of gold on vicinal Si surfaces are currently under intense discussion. Such structures can be investigated in microscopic detail by optical techniques such as Reflection Anisotropy Spectroscopy (RAS), which is extremely sensitive to the 1D nature of these systems. It will be shown that the local electronic properties of these surfaces can be tuned by controlled doping of hydrogen. The optical response of the clean Si(553), Si(553)-Au and hydrogenated Si(553)-Au surfaces are measured with RAS and compared with density functional theory (DFT) simulations. By analysing the optical response of the freshly prepared and hydrogenated Si(553)-Au surfaces, the spectral features can be directly attributed to specific atomic-scale structural elements on the surface. Hydrogen adsorption is shown to attenuate the response at spectral regions associated with the honeycomb chains at the Si step edges. The doping process is reversible and can be used as a controllable parameter to tune the electronic properties of this system.

O 19: Semiconductor Substrates: Structure, Adsorption and Growth

Time: Monday 17:00–19:30 Location: Poster A

O 19.1 Mon 17:00 Poster A

Epitaxial Growth of Ultrathin Lead Films on Silicon (111) — •Tobias Witte, Tim Frigge, Bernd Hafke, Boris Krenzer, and Michael Horn-von Hoegen — Department of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Epitaxial growth of ultrathin Pb films on Si(111) was studied by means of high resolution electron diffraction (SPA-LEED). The $\beta(\sqrt{3}\times\sqrt{3})$ reconstruction with 1/3 ML Pb-coverage ($1\,\mathrm{ML} \mathrel{\widehat{=}} 1$ Pb atom per Si surface atom $= 7.84 \times 10^{14}$ Pb atoms/cm^2) was prepared by desorption of a larger amount of Pb at 450 °C and used as a template layer for deposition. The layer-by-layer growth mode of Pb for coverages larger than 3 ML was confirmed through LEED intensity oscillations during deposition at low temperatures of 100 K. In the coverage regime of 1-3 ML the diffracted intensity is strongly reduced, indicating roughening of the strained Pb film. Films with 3-5 ML thickness are laterally relaxed through a network of interfacial misfit dislocations which is observed through satellite spots surrounding all integer order spots in the diffraction pattern. A $G(S)$-analysis indicates an increased vertical layer distance of 3.05 Å, which relaxes towards the bulk-like value of 2.87 Å for films of 6 or more ML thickness. This behavior is corroborated through the LEED intensity oscillations during deposition, which were measured at different diffraction conditions (i.e. different electron energies). Films deposited on the $\beta(\sqrt{3}\times\sqrt{3})$ reconstruction exhibit a slight azimuthal disorder, which is reflected through banana-like distorted integer order spots in the diffraction pattern. These films are metastable and form islands at temperatures above 220 K.

O 19.2 Mon 17:00 Poster A

Growth, structure and morphology of NiGe and SnGe nanostructures on Ge(001) — •Nicolas Braud[1], Simon Fischer[1], Inga Heidmann[1], Thomas Schmidt[1], Jan Ingo Flege[1], Tomasz Grzela[2], Thomas Schroeder[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Leibniz Institute of Innovative Microelectronics (IHP), Frankfurt (Oder), Germany

Nickel germanide is a promising candidate as a contact material in MOSFETs and is expected to play an important role in future Ge-based electronics due to its low formation temperature and low resistivity. In this context, SnGe can be used as channel material to improve the CMOS performance, as it has an even higher carrier mobility than Ge. Here we present an in-situ investigation of the growth of nickel germanide and SnGe at various temperatures on the Ge(001) surface by means of low-energy electron microscopy (LEEM) and micro diffraction (μLEED). We observe the growth of compact and elongated islands along two orthogonal directions after nickel deposition at 450°C and 530°C. We also show that with increasing temperature, the size of the NiGe islands increases while the island density drastically decreases, showing an Arrhenius like behavior [1]. Subsequent thermal annealing above 600°C results in the dissolution of the NiGe islands into the bulk substrate. Finally we compare the results obtained with the NiGe and those obtained with SnGe.

[1] *T. Grzela et al.*, Nanotechnology **26**, 385701 (2015)

O 19.3 Mon 17:00 Poster A

Hydrogen etching of SiC(0001): STM study of an epitaxy template — •Maximilian Bauernfeind, Felix Reis, Stefan Glass, Julian Aulbach, Ralph Claessen, and Jörg Schäfer — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

The hexagonal (0001) surface of silicon carbide (SiC) offers a huge playground for the epitaxy of a large variety of different materials, which has received little attention until now. One challenging aspect is the growth of high-Z atom lattices made out of, e.g., Sn or Bi in the monolayer regime, which may potentially form graphene analogs with a hexagonal structure. Because of the strong spin-orbit coupling in this class of materials, topological protected edge states can emerge. To enable epitaxy of such promising high-Z materials, one has to focus on the substrate quality, and prepare defect-free and well-ordered flat surfaces. In-situ gas phase etching can thereby attack the inert SiC much better than chemical pathways. It is performed at temperatures above 1000 °C in a hydrogen atmosphere.

To get new insights of this substrate on the atomic scale, we will address in general the differences between the etching treatments in a stationary and a flowing hydrogen atmosphere by means of scanning tunneling microscopy. To be specific, we will demonstrate the effects of different hydrogen flow values, including addition of the inert gas helium, as well as the influence of the substrate temperature. The results will be analyzed regarding large-scale terrace formation and defect density.

O 19.4 Mon 17:00 Poster A

Growing mechanism and tip-induced switching of acetylbiphenyl on Si(100)-(2x1):H — •Frank Eisenhut[1], Justus Krüger[1], Anja Nickel[1], Xavier Bouju[3], Gianaurelio Cuniberti[1,2], and Francesca Moresco[1] — [1]Institute for Materials Science, Max Bergmann Center of Biomaterials, and Center for Advancing Electronics Dresden, — [2]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany — [3]CNRS, CEMES (Centre d'Elaboration des Matériaux et d'Etudes Structurales), Toulouse, France

The investigation of molecules on semiconducting surfaces has caused much effort and can push forward molecular electronic devices. In this context one approach is to exploit the structure and related properties of the molecules and to use them as electronic components. In this study one candidate for a molecular latch, acetylbiphenyl (ABP), was investigated by means of low-temperature scanning tunneling microscopy on the passivated silicon surface. Firstly here we report on the growing mechanisms of ABP on Si(100)-(2x1):H. The molecule is fulfilling a dangling bond initiated growing mechanism along as well as perpendicular to the silicon dimer rows and consequently it is forming a 1-dimensional molecular assembly. Despite the growing of the molecule we found a reversible tip-induced conformational change of a molecule at the end of the grown molecular chain. This molecular change can be possibly used as a switch on this surface.

O 19.5 Mon 17:00 Poster A

Real-space investigation of the reaction channels of acetylene on Si(001) — Patrick Kirsten, •Christian Länger, and Michael Dürr — Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, 35392 Giessen

Ethylene and acetylene adsorption on Si(001) are benchmark systems for the understanding of adsorbate reactions on semiconductor surfaces. In the case of ethylene, the [2+2] cycloaddition proceeds via a mobile precursor state; in the final state the ethylene molecule is adsorbed either on top of one dimer or bridging two neighbored dimers of one dimer row. Due to different conversion barriers from the precursor into the final state, the on-top configuration is favored by a factor of ten at room temperature [1]. Early experiments on acetylene adsorption also report a precursor-mediated reaction channel [2]. On the other hand, DFT calculations suggest the existence of a direct reaction pathway for C_2H_2 on Si(001) [3].

In order to resolve this contradiction, we performed STM measurements after adsorption of acetylene at different surface temperatures. The ratio of on-top to end-bridge configurations is found to depend on surface temperature. From the temperature dependence, a precursor-mediated reaction is concluded and the barrier difference for the two reaction channels is calculated.

[1] Mette, et al., Chem. Phys. Lett. **483**, 209 (2009).
[2] Clemen, et al., Surf. Sci. **268**, 205 (1992).
[3] Cho and Kleinmann, Phys. Rev. B **69**, 075303 (2004).

O 19.6 Mon 17:00 Poster A

High Resolution Electron Energy Loss Spectroscopy of Ammonia Adsorbed on a Water Reacted Si(001)-(2x1)-Surface — Niklas Fornefeld[1], •Felicitas Scholz[1], Francois Rochet[3], Stefan Kubsky[2], and Ulrich Köhler[1] — [1]AG Oberflächenphysik, Ruhr-Universität Bochum, Germany — [2]Synchrotron Soleil, St. Aubin (Paris), France — [3]Laboratoire de Chimie Physique Matière et Rayonnement, Univ. P. et M. Curie, Paris, France

Surface bound hydroxyl-groups on silicon surfaces became an interesting topic for research due to their use as interface between an anorganic and an organic semiconductor. To investigate the binding properties (e.g. pKa-value) on those silanol-groups we studied the adsorption of ammonia (NH_3) as an example for a Lewis base. In order to verify the adsorption geometry and the behavior during the process of unfreezing, that had been proposed on the basis of XPS/NEXAFS studies, we studied the NH_3/(H/OH)/Si(001)-(2x1) system with HREELS at 125 K and 300 K. We report the self-limited adsorption of molecular ammonia on surface silanols in a proton-acceptor geometry (NH_3 giving lone pair to Si-OH) at 125 K. The saturation coverage was found to be smaller than one monolayer. In addition there were indications for the growth of a small amount of $SiNH_2$ (dissociation of NH_3) that seems to increase with higher dosage up to 17 L. At 300K (after unfreezing) the molecularly bound ammonia completely desorbs due to weak bonding while the behavior of $SiNH_2$ could not finally be cleared up.

O 19.7 Mon 17:00 Poster A

Sub-surface Incorporation of 3*d* Metal Atoms Into Bi(111) Films — •N.J. Vollmers[1], C. Klein[2], G. Jnawali[2], D. Lükermann[3], C. Tegenkamp[3], H. Pfnür[3], M. Horn-von Hoegen[2], W.G. Schmidt[1], and U. Gerstmann[1] — [1]Theoretische Physik, Universität Paderborn — [2]Fakultät für Physik, Universität Duisburg-Essen — [3]Institut für Festkörperphysik, Leibniz Universität Hannover

Substrate-stabilized Bi(111) bilayers and Bi(111) surfaces have been studied intensively due to the occurrence of strongly spin-orbit split surface states. The Bi(111) surface provides a well-defined incorporation site in the first bilayer that traps highly coordinating atoms like transition metals (TMs) or noble metals [1].

Here we use density functional theory (DFT) to gain a microscopic insight into the sub-surface incorporation and its implication for the Bi surface electronic properties. The Quantum-ESPRESSO package is used for relativistic DFT calculations. Thereby, spin-orbit coupling effects are included by using a numerically efficient PAW-based implementation [2]. It is found that 3*d* TMs penetrate the surface barrier-free, thereby causing no morphological changes at the surface. Isolated atoms assume a seven-fold coordinated interstitial position, and provide metallic near-surface state. Furthermore, we investigate the interaction between these subsorbates by analyzing subsorbate densities up to one impurity per Bi(111) unit cell. Interestingly in comparison to the single impurity, the Bi(111) lattice is restored to its ideal form.

[1] C. Klein et al., Phys. Rev. B 91, 195441 (2015).

[2] U. Gerstmann et al., Phys. Rev. B 89, 165431 (2014).

O 20: Tribology: Surfaces and Nanostructures

Time: Monday 17:00–19:30 Location: Poster A

O 20.1 Mon 17:00 Poster A

Preparation of structurally lubricated crystalline Au nanoparticles on HOPG for investigations on the shape and orientation dependence of sliding friction — •Felix Hartmuth, Matthias Vorholzer, Dirk Dietzel und André Schirmeisen — Institute of Applied Physics, Justus Liebig University Giessen, Germany

The widely acknowledged fundamental concept of structural lubricity explains the phenomenon of unusually low friction between two clean, rigid, and atomically flat surfaces with a structural surface mismatch that occurs due to incommensurate lattice parameters with regard to the sliding direction. Recent experiments and theoretical studies on structurally lubricated nanoparticles imply that besides the general lattice structure, the particle shape and orientation are also crucial key factors for the determination of sliding friction [1][2]. Since slightest particle rotation can already influence the interfacial friction, validating these concepts requires well defined nanoparticles and high-precision manipulation schemes. Therefore an improved manipulation procedure that allows in situ switching between FM NC-AFM and contact AFM has been set-up. First results obtained using gold nanoparticles on HOPG show that friction does indeed sensitively depend on the particle orientation. Further analysis will concentrate mainly on the switch in and out of pseudo-commensurate orientations.

[1] Dietzel et al., Phys. Rev. Lett. 111 (2013)

[2] de Wijn et al., Phys. Rev. B 86 (2012)

O 20.2 Mon 17:00 Poster A

Surface oxidation of metallic glass surfaces and its effect on nanotribology — •Kai Rittgen[1,2], Arnaud Caron[3], and Roland Bennewitz[1,2] — [1]INM Leibniz-Institute for New Materials, Campus D2.2, 66123 Saarbrücken, Germany — [2]Department of Experimental Physics, University of Saarbrücken, 66123 Saarbrücken, Germany — [3]Korea University of Technology and Education, Department of Energy, Materials and Chemical Engineering, Chungcheongnam-do, 31253 Republic of Korea

Owing to their high strength and hardness metallic glasses have been recognized as potential materials with enhanced wear resistance for tribological applications. While metallic glasses are prone to oxidation, the formation of surface oxide and its impact on tribological properties has been scarcely investigated. In this work we use a correlative approach to determine the influence of surface structure and chemistry on the friction and wear of metallic glass surfaces. Surface structural properties of several different metallic glasses are investigated by AFM in ultra high vacuum after Ar-sputtering and controlled oxidation treatments. Surface oxides are further characterized by SEM, TEM, and XPS. The tribological response of metallic glass surfaces with and without oxide layer is determined by AFM- and nano-scratching in air and in ultra high vacuum. Sputtered and oxidized surfaces of metallic glasses and their crystalline counterparts were compared to determine the relevant physical processes in wear mechanisms.

O 20.3 Mon 17:00 Poster A

Study of Nano Particle Interaction Force of Various Material Systems Using Atomic Force Microscopy — •Irina Schrezenmeier[1], Daniel Geiger[1], Clara Wanjura[1], Matthias Roos[2], Eugen Foca[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University — [2]Cleaning Technology Analytics, Carl Zeiss SMT GmbH

The use of nano particles in todays applications and the understanding of their characteristics is of utmost scientific and technological interest. One of these characteristics that needs further attention is the interaction force of nano particles with different substrates. We found that the interaction force of silica particles on silicon substrate shows aging phenomena. The force increases with time and parameters like humidity and temperature influence it as well. The aim of this work is to extend the measurements to the interaction force of various material combinations, such as aluminium particles on aluminium substrates, as well as combinations of aluminium with silica particles and silicon substrates. Further it is investigated if the roughness of the substrate's surface has an influence on the interaction force of the particle to this surface. Measuring this force is done by lateral atomic force microscopy (AFM). Thereby the particle is moved in contact mode AFM, where the torsion of the cantilever gives the force excerted on the particle. The trajectory of the particle is then recorded by imaging the sample in tapping mode AFM before and after the displacement.

O 20.4 Mon 17:00 Poster A

Energy Dissipation Mechanisms in Layered Structures — •Dilek Yildiz, Marcin Kisiel, and Ernst Meyer — Universität Basel

Bodies in relative motion separated by few nanometers gap experiences a tiny friction force. Although nature of non-contact friction is not fully understood yet, it can be measured by highly sensitive cantilever oscillating like a tiny pendulum over the surface. We investigate non-contact friction between Atomic Force Microscope (AFM) tip and the surface of TaS2 and Highly Oriented Pyrolytic Graphite (HOPG) crystals. Both samples are layered crystals with weak interaction between the layers. Yet, the origin of dissipation due to tip - sample interaction is different. While electrostatic type of dissipation is observed to be dominant on TaS2 surface, this type of dissipation is absent on HOPG surface. Interest of this study is to observe frictional response of TaS2 and HOPG to understand the dissipation mechanism in layered structures depending on their surface structures.

O 21: Morphology Prediction at Interfaces: Theory meets Experiment

Time: Monday 18:15–20:30 Location: Poster E

O 21.1 Mon 18:15 Poster E

Simulating stencil lithography of C60 growth: Impact of localized deposition — •B. Hartung, N. Kleppmann, and S. H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

Understanding and controlling the assembly of crystalline structures of complex organic molecules is an important aspect of the manufacturing of efficient organic and organic/inorganic hybrid semiconductor devices. In organic molecular beam epitaxy growth scenarios, the structure formation can be manipulated by using stencil masks to restrict the molecular beam to a certain area of the substrate. This technique is known as stencil lithography. To examine the basic effects of the mask on the growth behavior of organic molecules, we use C60 homoepitaxy as a model system, based on previous studies [1, 2]. To this end we perform Kinetic Monte Carlo simulations, where the adsorption of particles is restricted to a quadratic area, which is small compared to the size of the overall substrate surface.

The growth behavior shows a transition from the formation of multilayer-islands (covering only the surface of the deposition area) to the formation of monolayer-like islands, the control parameters being the temperature and the adsorption rate. We discuss this behavior studying layer coverages and geometric aspects of growth.

[1] S. Bommel, N. Kleppmann et al., Nat Comm 5, 5388 (2014), doi:10.1038/ncomms6388

[2] N. Kleppmann, S. H. L. Klapp, J. Chem. Phys. 142, 064701 (2015)

O 21.2 Mon 18:15 Poster E

Naphthalene‘s six shades on graphite — •Falko Sojka[1], Matthias Meissner[1], Takashi Yamada[2], Toshiaki Munakata[2], Roman Forker[1], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Department of Chemistry, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

Naphthalene ($C_{10}H_8$) is the smallest member of the polycyclic aromatic hydrocarbons (PAH). For $C_{10}H_8$ two commensurate monolayer phases on graphite have been reported so far. By using low energy electron diffraction (LEED) we re-analyze precisely the lattice parameters of these systems. Surprisingly, we found a total of six different phases of which only one exhibits an ordinary commensurate registry with graphite. Two further phases vanish irretrievably upon a change in the temperature, while the other three can be converted into one another reversibly. We studied in detail how to obtain the different phases by varying the amount of molecules deposited as well as the substrate temperature. Eventually, the complex behavior and polymorphism of $C_{10}H_8$ on graphite is compiled in a phase diagram. We believe that such manifold systems should be taken into consideration for theories which try to predict structures and morphologies of adsorbates on surfaces.

O 21.3 Mon 18:15 Poster E

Investigation of the lateral and vertical structure of CuPc on Cu(001) — •Markus Franke, Sonja Schröder, Jonas van Bebber, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich GmbH, Jülich, Germany, and Jülich-Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

For thin molecular films adsorbed on metal surfaces it has been shown that morphology has a big influence on the electronic properties of the system. To achieve a better understanding of the formation of ordered structures, we investigated the system Copper-II-phthalocyanine (CuPc) on Cu(001).

Depending on the substrate temperature and the (sub-monolayer) coverage the CuPc molecules form several different commensurate structures or, at low coverages, remain disordered. We characterized these different phases using STM and LEED, and in one case also with XSW. The most remarkable result may be the breaking of the fourfold symmetry of the LUMO in one of the structures, caused by the degeneracy of both LUMO states being lifted upon adsorption. This is surprising, since both the Cu(001) substrate and the adsorbed molecules originally have the same (fourfold) symmetry.

O 21.4 Mon 18:15 Poster E

Free-Base 5,10,15-tris(pentafluorophenyl)corrole adsorption on Ag(111) — •Hazem Aldahhak[1], Stefano Tebi[2], Mateusz Paszkiewicz[3], Eva Rauls[1], Uwe Gerstmann[1], Stefan Müllegger[2], Florian Klappenberger[3], Wolfgang Schöfberger[4], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn — [2]Festkörperphysik, Universität Linz — [3]Physik Department E20, Technische Universität München — [4]nstitut für Organische Chemie, Universität Linz

While corroles are structurally closely related to porphyrins, they have lower symmetry, smaller cavities, which enables them to stabilize metal ions in exceptionally high oxidation states. This makes them highly interesting for a variety of applications in medicine, catalysis, sensors as well as for solar cells.

Here, dispersion-corrected density-functional theory (DFT) calculations supported by scanning tunneling microscopy (STM) measurements and X-ray photoelectron spectroscopy (XPS) measurements on the adsorption of the free-base 5,10,15-tris(pentauorophenyl)corrole on Ag(111) surface are presented. Both, single adsorbed molecules as well as monolayer thin films are studied. Single molecules adsorb with its macrocycle tilted with respect to the surface. The tilted adsorption geometries enable the molecules to aggregate in non-trivial interwoven monolayer structures. The simulated STM data as well as the simulated X-ray photoelectron spectroscopy (XPS) data for the C1s, F1s and N1s edges in conjunction with the measurements nicely confirm the molecular structures concluded from the total-energy calculations.

O 21.5 Mon 18:15 Poster E

Behaviour of the water lithium niobate interface studied from first principles — •Rebecca Hölscher, Simone Sanna, and Wolf Gero Schmidt — Paderborn University

Lithium niobate ($LiNbO_3$, LN) is a frequently used material for optical and acoustic applications due to its strong piezoelectric, pyroelectric, and photorefractive properties. As for other ferroelectric materials, manipulating the polarization can change the surface reactivity. This opens the possibility for the realization of molecular detectors and other devices [1]. The water lithium niobate interface is largely unknown. Moreover, recent results show that basic properties of water such as the freezing temperature are strongly polarization dependent [2]. We present here ab initio calculations on the adsorption of water films on both the positive and the negative Z-cut and the X-Cut surface of LN. The adsorption is modelled by means of density functional theory (DFT) within the generalized gradient approximation [3,4]. The interface atomic structure and dynamics are calculated using Molecular Dynamic simulations at room temperature. The influence of the surface polarity on the water layer is investigated by means of a correlation function analysis.

[1] D. Li, et al., Nature Materials **7** (2008) 473.

[2] D. Ehre et al., Science **327** (2010) 672.

[3] W.G. Schmidt, et al., Phys. Rev. B **77** (2008), 035106.

[4] S. Sanna, A.V. Gavrilenko, W.G. Schmidt, Phys. Stat. Sol. C **7** (2010) 145.

O 21.6 Mon 18:15 Poster E

Molecular Structures of Dialkylimidazolium Ionic Liquids at the Hydroxylated Solid-Liquid Interface — •Michael Klimczak[1], Zlatko Brkljača[2,3], David M. Smith[2,3], Ana-Sunčana Smith[2,3,4], and Andreas Magerl[5] — [1]Chair of Crystallography and Structural Physics, FAU, Erlangen, Germany — [2]Division of Organic Chemistry and Biochemistry, Institut Ruđer Bošković, Zagreb, Croatia — [3]Cluster of Excellence Engineering of Advanced Materials, FAU, Erlangen — [4]Institute for Theoretical Physics I, FAU, Erlangen, Germany — [5]Chair of Biophysics, FAU, Erlangen, Germany

Dialkylimidazolium-based ionic liquids, salts with a melting point well below room temperature, are a fairly novel class of substances with a broad spectrum of potential applications, most notably as solvents or electrolytes in an electrochemical context. Molecalar structuring at the solid liquid interface, oftentimes playing a crucial role in small-scale systems, has previously been observed. Yet, no coherent explanation has been given to provide a better understanding of these phenomena.

Using a complementary approch of experimental X-ray reflectivity and molecular dynamics, we obtain atomic level detail of structuring at the solid-liquid interface of 1-alkyl-3-methylimidazolium bistriflimide ionic liquids. The interface region is dominated by cations, tightly attached to the substrate via hydrogen bonding and a two-dimensional long-range ordering can be observed. This structure is followed by interface normal, monomolecular layering of alternating anion and cation enrichment/depletion, extending about 40 Å into the bulk.

O 21.7 Mon 18:15 Poster E

Ab initio electron paramagnetic resonance study of 3C-SiC/SiO2 interfaces in SiC-nanofiber based solar cells — •Taufik Adi Nugraha[1,2], Uwe Gerstmann[2], Wolfgang Gero Schmidt[2], and Stefan Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung, Germany — [2]University of Paderborn, Germany

Semiconducting nanocomposites, e. g. hybrid materials based on inorganic semiconducting 3C-SiC nanofibers and organic surfactants, provide genuinely novel pathways to exceed the Shockley-Queisser limit for solar energy conversion. The synthesis of such functionalized fibers can be performed completely using only inexpensive wet chemical solution processing. During synthesis a thin passivation layer is introduced between the SiC-fiber and surfactants, e. g. the native oxide, whose atomistic details are poorly understood. In this study, we utilize unpaired spins in interfacial defects to probe the local chemical environment with ab initio EPR (Electron Paramagnetic Resonance) calculations, which can be directly compared to experiment. Considering a wide variety of possible interfacial structures, a grand canonical approach is used to generate a phase diagram of the 3C-SiC/SiO2 interface as a function of the chemical potentials of Si, O and H, to provide favorable interfacial structures for g-tensor calculations. This study provides directions about specific types of interfacial defects and their impact on the electronic properties of the interface. The authors wish to thank S. Greulich-Weber for helpful discussions.

O 21.8 Mon 18:15 Poster E

Vibrational properties of Pb/Si (111) from first principles — •Maedeh Zahedifar and Peter Kratzer — Faculty of Physics,University of Duisburg-Essen,Germany

Time-resolved spectroscopic methods hold great potential for the exploration of electronic properties of materials. However, the electronic excitation and relaxation processes are, due to their complexity, incompletely understood at present. Due to their unique electronic properties, ultra-thin metallic films on semiconductor surfaces are an important field of contemporary solid state physics. In particular, we studied Pb metallic films of a few monolayers on silicon as substrate in (111) direction. The quantum well states in these films are ideally suited to study electronic relaxation by time-resolved spectroscopy. Therefore, we employed density functional calculations using the GGA-PBE functional to study various structures of Pb/Si(111) and their stabilities. In our calculations using the Quantum-Espresso and the VASP code, we tested different unit cells: 1×1, $\sqrt{3}\times\sqrt{3}$ and $\sqrt{7}\times\sqrt{3}$ for 1ML, and $\sqrt{3}\times\sqrt{3}$ for 4 and 5ML. We find that the system in $\sqrt{3}\times\sqrt{3}$ is more stable than in the other structures. The optical in-plane modes at Pb $\sqrt{7}\times\sqrt{3}$ are somewhat lower in energy than those of Pb $\sqrt{3}\times\sqrt{3}$, in agreement with Raman scattering experiments. That is because the density of the Pb layer in $\sqrt{7}\times\sqrt{3}$ is less than in the $\sqrt{3}\times\sqrt{3}$, expressed as coverage 1.2 ML versus 1.333 ML. Calculations are in progress addressing the electron-phonon coupling.

O 22: Organic-Inorganic Hybrid Systems and Organic Films

Time: Monday 18:15–20:30 Location: Poster E

O 22.1 Mon 18:15 Poster E

Ordered films of the charge-transfer salt DTBDT-F4TCNQ on Au(111) — •Torge Mashoff and Hans-Joachim Elmers — Institut für Physik, Johannes Gutenberg-Universität, Mainz

The interplay of electronic correlation effects with low dimensionality and geometric frustration of charge-transfer compounds provides a large playground for variable many-body interactions. Novel systems of molecules with tailored donor and acceptor character provide a vast multitude of possible modifications. Understanding the electronic structure of this class of materials as well as their metal-organic interfaces is crucial for designing specific electronic properties. An important precondition for the implementation of organic charge-transfer salts in electronic devices is the fabrication of thin films with appropriate molecular orientation. Deposition of films under ultrahigh vacuum (UHV) conditions promises the formation of well-defined interfaces [1]. In this work, an in-situ prepared molecular monolayer of the novel charge-transfer salt dithienobenzodithiophene-tetrafluorotetracyanoquino-dimethane (DTBDT-F4TCNQ) has been deposited on a gold substrate and investigated by low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS), allowing the characterization of occupied and unoccupied electronic states of the donor-acceptor compounds near the Fermi level. [1] D. Bayer et. al., Phys. Rev. B 89, 075435 (2014)

O 22.2 Mon 18:15 Poster E

Substrate-directed growth of aromatic molecules on a metal surface — •Friedrich Maass[1], Arnulf Stein[1], Bernd Kohl[2], Lena Hahn[3], Lutz H. Gade[3], Michael Mastalerz[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Organisch-Chemisches Institut — [3]Anorganisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Germany

The influence of the substrate on the adsorption behaviour of π-conjugated molecules on metal surfaces is of immense interest for understanding the structural and electronic properties of small molecule organic semiconductors.

We investigated the adsorption geometry and the electronic properties of benzene, pentacene, 1,3,8,10-tetraazaperopyrene (TAPP) and quinoxalino[2',3':9,10]phenantro[4,5-abc]-phanzine (QPP) on the Au(111) surface with vibrational and electronic high-resolution electron energy-loss spectroscopy (HREELS), thermal-programmed desorption (TPD), and density functional theory calculations. In all cases we found a clear difference between the structure of thin-films and the bulk-structure obtained by X-ray structure analysis.[1] While in the bulk all molecules show a herringbone like orientation with π-stacked molecules and angles ranging from 35 to 90° between the molecular planes in neighbouring stacks, we observe planar adsorption on the surface for the monolayer (ML) as well as for higher coverages (up to 10 ML).

[1]L. Hahn, F. Maass *et al.*, *Chem. Eur. J.* **2015**, *21*, 17691.

O 22.3 Mon 18:15 Poster E

Studying the F4TCNQ/Au(111) Interface with Two-Photon Photoemission — •Sascha Feldmann, David Gerbert, and Petra Tegeder — Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Deutschland,

In our ongoing efforts pointing towards a deeper understanding of the electronic properties at metal/organic interfaces a convenient approach could be the characterization of well-studied organic molecules adsorbed on single crystal noble metal surfaces. Tetrafluorotetracyanoquinodimethane (F4TCNQ) adsorbed on Au(111) was chosen as a prototypical system to investigate a negatively charged organic acceptor molecule on a noble metal surface by means of two-photon photoemission (2PPE). 2PPE enables the observation of occupied and unoccupied electronic states as well as the study of photo-induced processes via photo-induced changes in the electronic structure. Varying photon energies, angle of incidence or time delay between two laser pulses further information about dispersion and lifetime of electronic states can be obtained, resulting in a detailed picture of the electronic properties of the F4TCNQ/Au(111) interface.

O 22.4 Mon 18:15 Poster E

A combined photoemission and LEED study of SnPc/Ag (111) — •Stephan Jauernik, Max Gurgel, Petra Hein, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

Recently, the adsorption of tin-phthalocyanine (SnPc) on Ag(111) has attracted considerable interest due to peculiarities in the adsorbate-substrate interaction [1] and switching capabilities reported for the adsorbed SnPc [2]. In a combined Low Energy Electron Diffraction (LEED) and Photoemission/Two-Photon Photoemission (PES/2PPE) study of SnPc/Ag(111) we address in this work the correlation of the structural and the electronic properties of this model system in the sub-monolayer coverage regime. The study focuses on the transition regime from a gas - like phase at coverages <0.90 monolayers (ML) to an incommensurate phase observed for coverages between 0.90 ML and 1.0 ML. The photoemission data reveal distinct changes in the occupied as well as unoccupied electronic structure of this model-type organic adsorption system as the coverage increases. The experimental results are discussed under consideration of past LEED, STM and STS studies [1,2].

[1] C. Stadler et al., Nature Physics 5, 153-158 (2009)

[2] Y. Wang et al., J. Am. Chem. Soc., 2009, 131 (10), 3639-3643

O 22.5 Mon 18:15 Poster E

Naphthalocyanine on metal surfaces studied with a variable temperature STM — •Malte Schulte, Ismail Baltaci, Patrick Mehring, and Carsten Westphal — Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany

The class of naphtalocyanine molecules received large attention within the recent years. In particular, the dependence of their geometric and electronic properties on the central metal ion causes high interest. Therefore, their adsorption and structural formation were determined in several studies. Especially their self-assembly on different surfaces was studied at room temperature.

In this study metal free naphtalocyanine (H2Nc) is investigated on metal surfaces at various low temperatures by scanning tunneling microscopy. STM imaging at low temperature allows to increase the resolving of single molecules. The coverage of the studied surface is less than a monolayer H2Nc while analyzing their self-assembly formation.

O 22.6 Mon 18:15 Poster E

A molecular ruler for measuring the mesoscopic relaxations in Co/Au(111) interfaces — •Zheng Wei[1,2], Jobynson Kollamana[1], Benjamin Stadtmüller[1], Mirko Cinchetti[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]College of Material Science and Engineering, Chongqing University, 400044 Chongqing, P. R. China

The contact between a molecular and ferromagnetic electrode contributes or even determines the performance of molecular spintronic devices. Here we report on scanning tunneling microscopy experiments on the C_{60}/Co/Au(111) system. We observed a disorder-order molecular transition at evaluated temperature of 620K, independent of the cobalt thickness. However, the ordered molecular superstructures depend on the thickness of cobalt, reflecting the lattice dilatation in cobalt and inter-diffusion of Au. This means that C_{60} is a sensitive molecular ruler to measure the mesoscopic relaxation of cobalt films on Au(111) substrate. Furthermore, our results suggest an alternative way to tailor the perpendicular magnetic anisotropy of Co/Au(111) interfaces besides the coverage of C_{60} [1].

[1] K. Bairagi et al., Phys. Rev. Lett. **114**, 247203 (2015).

O 22.7 Mon 18:15 Poster E

Temperature Dependent Structure Formation of Phthalic Acid on Cu (111) — •Feifei Xiang, Tobias Schmitt, Anastasia Sokolova, and M. Alexander Schneider — Solid State Physics, Friedrich-Alexander-University Erlangen-Nürnberg, Erlangen, Germany

Carboxylic acids are popular building blocks in molecular self-assembly and many examples show that deprotonation at surfaces changes the obtained structures. Here we investigate an example where surface-induced anhydride and poly-anhydride formation were found previously on a Ag(100) surface [1]. We studied the self-assembly of phthalic acid (1,2-Benzenedicaboxylic Acid) by low-temperature scanning tunneling microscopy on Cu(111) surface as function of the substrate temperature. At room temperature and above phthalic acid forms phthalic anhydride on Cu(111). However, contrary to the situation on Ag(100) [1], we find that monomers of phthalic anhydride are present on Cu(111) and form linear ribbon structures at room temperature. Our experiments also indicate that multilayer molecular packing is still stable at 423K. The extraordinarily ordered structures found finally decompose above 473K.

[1] M. Franke, et al. J. Phys. Chem. C, 2015, 119, 23580*23585

O 22.8 Mon 18:15 Poster E

In-situ Kelvin Probe Study of the Work Function Evolution of Molybdenum Oxide Upon Gas Exposure — Sebastian Hietzschold[1,2,3], Sebastian Beck[1,3], •Stefan Brackmann[1,2], Robert Lovrincic[1,2], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg, Germany — [2]Institute for High Frequency Technology, TU Braunschweig, Braunschweig, Germany — [3]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany

The electronic properties of transition metal oxides are very sensitive to many processing parameters. It is still not completely understood if just oxidative adsorption at the surface or also diffusion into bulk vacancies is the reason for the observed changes in the effective surface potential. To clearly separate surface from bulk effects, we measure simultaneously the bulk conductivity (via current-voltage measurements) and work function (via Kelvin probe) of MoOx layers of varying thicknesses in-situ during gas exposure.

We find that shortly after evaporation of thin MoOx onto a silicon substrate with native oxide the work function starts at a maximum of 6.9 eV and then decreases monotonously down to 5.7 eV for exposure with pure oxygen and well below 5 eV for air exposure. We observe the saturation of the work function change even for low exposure. We also show that the gradient of this decrease as well as the saturation value of the decreased work function does not only depend on the total exposure but also on the time of the exposure, the base pressure and gas species supplied during the exposure.

O 22.9 Mon 18:15 Poster E

Adjusting the Work Function of Solution Processed Nickel Oxide by Self-Assembled Monolayers — •Florian Friedrich[1,2], Sebastian Hietzschold[1,2,3], Patrick Reiser[1,4], Eric Mankel[1,4], Sabina Hillebrandt[1,2], Robert Lovrincic[1,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab, Heidelberg, Germany — [2]KIP, Heidelberg University, Germany — [3]IHF, TU Braunschweig, Germany — [4]MAWI, TU Darmstadt, Germany

Solution processed nickel(II) oxide (NiO) is a promising hole selective anode material in organic devices. However, the work function of NiO is too low for many currently used organic materials [1]. The purpose of this work is to adjust the work function of solution processed NiO thin films via self-assembled monolayers (SAMs). A few nanometer thin NiO layers, formed by monoethanolamine with nickel acetate tetrahydrate in ethanol, were spin-coated on an indium tin oxide (ITO) surface and were thermally annealed in ambient atmosphere. The effective surface work function of this NiO layers were adjusted by chemisorption of phosphonates in terms of dipolar SAMs such as perfluorohexyloctyl phosphonic acid. Work function changes were examined by Kelvin probe measurements and photoelectron spectroscopy. The surface has been further characterized with atomic force microscopy, ellipsometry and goniometry. The results can be used to improve energy level alignment at interfaces in organic opto-electronic devices and increase their overall efficiency. References: [1] Schulz et al., NiOX/MoO3 Bi-Layers as Efficient Hole Extraction Contacts in Organic Solar Cells. Adv. Funct. Mater., 24: 701-706 (2014)

O 22.10 Mon 18:15 Poster E

Energy-Level-Engineering of Indium-Tin-Oxide (ITO) - Linking Simulation and Experiment for Small Molecule Self-Assembled-Monolayers (SAMs) — •Johannes Breuer, Julia Rittich, Sebastian Mäder, Carolin C. Jacobi, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University

Organic electronics promise cost-effective and easy fabrication of highly energy-efficient and versatile devices. Over the last decade these prospects have motivated a vast variety of research activities. One of the major issues that still has to be addressed is the energy-level-mismatch at the critical electrode-organic interface.

Indium tin oxide (ITO) is a transparent conductive electrode-material that is crucial for the development of organic electronic applications like organic thin-film transistors (OTFTs) or organic light emitting diodes (OLEDs). Understanding and controlling the surface properties of ITO allows molecular engineering of the ITO organic interface which enables precise control of the interfacial chemistry and electronics. One way to optimize the energy-level alignment at the ITO interface is the use of monolayers based on organic molecules with tailored functional groups.

In this work the modified surfaces of ITO coated with self-assembled-monolayers (SAMs) are characterized by means of photoelectron spectroscopy, contact angle and kelvin probe measurements. Via gas-phase simulations of these organic molecules it is possible to link calculated properties and experimental results.

O 22.11 Mon 18:15 Poster E

Functionalization of Gallium nitride surfaces — •Stefan Brackmann[1,2,3], Sebastian Hietzschold[1,2,3], Robert Lovrincic[1,2], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab, Heidelberg, Germany — [2]IHF, TU Braunschweig, Germany — [3]KIP, Heidelberg University, Heidelberg, Germany

Gallium nitride (GaN) is an often used III-V semiconductor due to its favorable optoelectronic properties. GaN nanowires with different doping domains are a promising candidate for blue LEDs. However the material suffers from surface states that are detrimental to its electronic properties 1. One approach to mend the problematic surface states is passivation with different self-assembled monolayers (SAMs) such as amines, tiols and phosphonates. Here, we study GaN surfaces with atomic force microscopy (AFM), ambient Kelvin probe (KP), Surface photo voltage (SPV), UV-Vis spectroscopy and goniometry. Clean (0001) n-type GaN surfaces are compared with functionalized surfaces. Modification of the surface changed the work function as well as the SPV by several 100mV. We will discuss the impact of our surface functionalizations on the band diagram and charge carrier recombination.

1. Reshchikov, M. a., Visconti, P. & Morkoc*, H. Appl. Phys. Lett. 78, 177 (2001).

O 22.12 Mon 18:15 Poster E

Development of a New Update Mechanism for High Charge Carrier Densities in Kinetic Monte Carlo Simulations — •Markus Krammer[1], Chris Groves[2], and Karin Zojer[1] — [1]Institute of Solid State Physics and NAWI Graz, TU Graz, Austria — [2]School of Engineering and Computing Science, Durham University, United Kingdom

Kinetic Monte Carlo simulations (KMC) have become a widely used tool to get a better understanding of the behaviour of charge transport in organic semiconductors and devices [1]. With the help of such simulations, the transport-related properties of a system are derived from the trajectories of all particles hopping through a three-dimensional grid of sites as a function of individually chosen site properties.

Regarding the update mechanism, the Full Dynamic Monte Carlo Method (DMC) and the so-called First Reaction Method (FRM) [2] are currently established. Where DMC recalculates all rates after each step, FRM performs only a very local update. This leads to highly accurate results but high computational costs for DMC and fast simulations but imprecise results for FRM. Especially for high charge carrier densities, both methods are inappropriate. In this connection our new update method combines low computational cost and high accuracy. We present the performance of this improved update mechanism for bulk simulations as well as simulations of injection from a metal contact to an organic semiconductor.

[1] R. Kimber et al., Phys. Rev. B, 86, 235206 (2012)

[2] C. Groves et al., J. Chem. Phys., 133, 144110 (2010)

O 22.13 Mon 18:15 Poster E

DFT calculations on the etching of crystalline ZnO surfaces upon formation of phosphonic acid self-assembled monolayers — •Tobias Klöffel[1], Alexandra Ostapenko[2], Gregor Witte[2], and Bernd Meyer[1] — [1]Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg — [2]Fachbereich Physik, Philipps-Universität Marburg

Among the inorganic oxides, ZnO is of special interest for hybrid organic-inorganic interfaces in molecular electronics due to its high charge carrier mobility. However, in recent experiments it was observed that self-assembled monolayers of phenylphosphonic acids (PPAs), a typical representative for commonly used linker groups and functional organic units, are not stable but etch the ZnO substrate. Using density-functional theory (DFT) calculations we show that the origin of this instability is the unusual strength of the PPA–ZnO interaction together with a geometric misfit between the pi-stacking of the phenyl rings and the ZnO lattice constant. As a result, the transformation of PPA layers on ZnO to ZnPPA crystals becomes a thermodynamically favorable reaction. Our DFT calculations provide a first simplified reaction pathway for this transformation process.

O 22.14 Mon 18:15 Poster E

On the Adsorption Behavior of Ionic Liquid (Sub-)monolayers on Model Electrode Surfaces and their Interaction with Coadsorbed Lithium — •Florian Buchner[1], Katrin Forster-Tonigold[1], Maral Bozorgchenani[2], Bendikt Uhl[2], Axel Gross[1,3], and R. Jürgen Behm[1,2] — [1]Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, D-89081 Ulm, Germany — [2]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — [3]Ulm University, Institute of Theoretical Chemistry, D-89069 Ulm, Germany

Ionic Liquids (ILs) as 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide [BMP][TFSA] have become attractive candidates for battery electrolytes. In this model study we investigated the adsorption behavior of (sub-)monolayers of [BMP][TFSA] on metallic substrates and now also on graphite(0001) as frequently used anode material under ultrahigh vacuum (UHV) conditions, applying scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and dispersion corrected density functional theory (DFT-D) calculations. After vapor deposition at 300 K, XPS reveals a 1:1 ratio of cations : anions on Ag(111) and graphite(0001). Upon subsequent cool-down to 100 K, STM demonstrates ordered molecular arrangements, which clearly differ on both surfaces; a detailed comparison is given in terms of adsorption geometry, intermolecular and substrate-adsorbate interactions. In addition, we investigated the interaction with coadsorbed Li, which resulted in a decomposition of the ions. This will be discussed based on ongoing DFT-D calculations.

O 22.15 Mon 18:15 Poster E

Triplet emitters for OLEDs investigated by STM and STS — •Anne Bakker[1,2], Wu Xu[3], Sebastian Wilde[1,2], Shiyu Zhu[3], Haiming Guo[3], Shixuan Du[3], Hong Ying Gao[1,2], Hongjun Gao[3], Cristian Strassert[1,2], and Harald Fuchs[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Germany — [2]CeNTech, Westfälische Wilhelms-Universität, Münster, Germany — [3]Institute of Physics, Chinese Academy of Sciences, Beijing, China

Pt(II)-triplet emitters are promising candidates for application in OLEDs. The heavy-metal atom with its large spin-orbit coupling enables emission via triplet states with high phosphorescence quantum yield. In previous work it has been shown that the HOMO-LUMO gap of such emitters can be tuned by adjusting the substituents in the periphery of the luminophoric pincer ligand coordinated to the metal centre [1,2].

Here we study the self-assembled nanostructures and electronic properties of a series of new triplet emitters by low-temperature scanning tunnelling microscopy and spectroscopy. In our case the metal-organic complex contains a platinum d8 cation and a tetradentate ligand. To systematically investigate the influence of different electron-withdrawing side groups on the alignment of the energy levels, ligands with 0, 2, 4, and 6 Fluor atoms are used. Our experiments can provide insight in the behaviour of Pt(II)-complexes on surfaces and the possibilities to specifically design new triplet emitters.

[1] P.R. Ewen et al., Physcal Review Letters 111, 267401, (2013)

[2] J. Sanning et al., Angewandte Chemie 54, 786-791, (2015)

O 22.16 Mon 18:15 Poster E

Impact of a MoO_3 front contact buffer layer on the electric and interface properties in organic bilayer solar cells — •Patrick Reiser[1,4], Michael Scherer[2,4], Sabina Hillebrandt[3,4], Robert Lovrincic[2,4], Wolfgang Kowalsky[2,4], Sebastian Beck[3,4], Annemarie Pucci[3,4], Eric Mankel[1,4], and Wolfram Jaegermann[1,4] — [1]Institute of Materials Science, Technische Universität Darmstadt — [2]Institut für Hochfrequenztechnik, Technische Universität Braunschweig — [3]Kirchhoff-Institut für Physik, Universität Heidelberg — [4]InnovationLab GmbH, Heidelberg

In this study we correlate the chemical and electronic interface properties at different front contacts of conventional F_4ZnPc:C_{60} bilayer solar cells with their electric characteristics. Starting from device and Scanning Kelvin Probe Microscopy data, we examine the interface of ITO/MoO_3/F_4ZnPc and ITO/F_4ZnPc using Photoelectron Spectroscopy on subsequently deposited layers of F_4ZnPc. As oxide substrates we used O_2-plasma cleaned ITO on glass and the same ITO coated with a 10nm thick intermediate MoO_3 buffer layer which shows a significant higher work function than bare ITO. There is a moderate impact of the buffer layer on the electronic band alignment difference of about 100meV. However, we observe chemical interactions of the F_4ZnPc with the ITO substrate. In-situ IR spectroscopy measurements were performed to study the F_4ZnPc adsorption mechanisms on differently treated oxide surfaces. Finally, the analytical measurements could successfully be correlated with the electric characteristics of the solar cell device.

O 22.17 Mon 18:15 Poster E

The OTFT Awakens - Live in-situ organic thin film transis-

tor (OTFT) measurements during growth — •Nils Norrman, Sebastian Mäder, Julia Rittich, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University

Organic semiconductors are of great interest for optoelectronic applications due to their high flexibility and efficiency. Indeed, first commercial products are already available like OLED displays and organic solar cells. The investigation of organic thin film transistors (OTFTs) provides a peerless opportunity for understanding the crucial properties influencing the electrical performance.

Here, we present live in situ measurements obtained during the growth of the very first layer of the organic-channel-material. The OTFTs were prepared using a bottom gate bottom contact geometry to enable electrical contacting during thermal evaporation of the organic material. Precisely controlling deposition rate and substrate temperature in a special vacuum setup allows to electrically characterize all critical properties right from the moment the first molecules arrive at the substrate.

These properties provide an excellent insight into the underlying effects governing efficiency in organic materials.

O 23: Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy

Time: Monday 18:15–20:30 Location: Poster E

O 23.1 Mon 18:15 Poster E

Time of flight momentum microscopy of plasmon assisted photoemission — •Martin Lehr[1], Karina Bley[2], Nicolas Vogel[2], Gerd Schönhense[1], and Hans Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55122 Mainz — [2]Friedrich-Alexander University Erlangen-Nürnberg, 91058 Erlangen

The photoemission properties of a Au nano triangular array have been investigated using a time-of-flight-momentum microscope (ToF-PEEM), equipped with a state-of-the-art Surface Concept delay line detector (DLD). The nano triangular array has been fabricated by deposition of a gold film on a self-assembled colloidal sphere structure. The triangles can be resonantly excited by Ti:sapphire femtosecond laser pulses. The sample is illuminated from the backside at normal incidence. We have studied the photoemission intensity as a function of kinetic energy and parallel momentum. Both dependencies deviate from results obtained for flat surfaces.

O 23.2 Mon 18:15 Poster E

Excitation of Surface Phonon Polaritons using an Infrared Free-Electron Laser — •Nikolai Passler, Ilya Razdolski, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Similar to surface plasmon polaritons (SPPs) at metal surfaces, polar dielectrics can support surface polaritons. These surface phonon polaritons (SPhPs) [1] emerge due to negative permittivity between transverse and longitudinal optical phonon frequencies, the so-called Reststrahl region. As for SPPs, these excitations are non-radiative due to a wave vector mismatch, which is why they can only be excited in sub-wavelength nanostructures or via prism coupling. SPhPs have, however, much longer lifetimes than SPPs, promising low-loss optical modes below the diffraction limit.

Here, we employ the Otto geometry [2] for prism coupling to excite SPhPs at the SiC-air interface, using a tunable mid-infrared Free-Electron Laser (FEL). In this configuration, the necessary momentum for SPhP excitation is provided by the evanescent wave leaking into the air gap between prism and sample for incident angles of total internal reflection inside the prism. The optimal coupling conditions for the phase-matched SPhP excitation are studied using reflectance spectroscopy. Additionally, the resonant nonlinear response of the excited SPhPs is probed by second harmonic generation spectroscopy.

[1] Neuner et al., Opt. Lett. 34, 2667 (2009)
[2] Otto, Zeitschrift für Physik 216, 398 (1968)

O 23.3 Mon 18:15 Poster E

Upconversion of infrared free-electron laser light in gallium selenide — •Riko Kiessling, Sandy Gewinner, Wieland Schöllkopf, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der MPG, Berlin

For absolute timing synchronization with sub-picosecond accuracy between table-top and accelerator-based free-electron lasers (FELs), it is essential to develop efficient schemes for relative timing measurements [1]. Specifically, for the synchronization between an FEL tunable throughout the mid-infrared frequency region [2] and a near-infrared table-top laser, light upconversion by sum-frequency generation could provide sufficient sensitivity for online-timing measurements.

As a first step, we have investigated the sum-frequency generation in gallium selenide by mixing the picosecond FEL pulses with near-infrared nanosecond pulses from a Nd:YAG laser. The conversion process is explored in terms of phase-matching and azimuthal angle dependence, polarization orientations and intensity scaling over a broad spectral range, utilizing the tunability of the FEL. Gallium selenide presents itself as an efficient nonlinear medium in the infrared, allowing its application to determine the absolute timing between the FEL and femtosecond table-top laser pulses.

[1] S. Schulz et al., Nat. Commun. 6, 5938 (2015)
[2] W. Schöllkopf et al., Proc. SPIE 9512, 95121L (2015)

O 23.4 Mon 18:15 Poster E

Incident Angle-Tuning of Infrared Antenna Array Resonances for Molecular Sensing — •Andreas Hessler, Tobias W.W. Mass, and Thomas Taubner — Institute of Physics (IA) RWTH Aachen

Metallic structures can efficiently couple light into a region of subwavelength size. In these regions, large local field enhancements can occur and enable an increased absorption of molecules which are placed in these so called "hot spots". Arrays of metallic structures which are designed for surface enhanced infrared absorption spectroscopy (SEIRA) enable the detection of molecular vibrations with high sensitivity [1,2].

In recent work [3], we apply incident angle-tuning to antenna array resonances in order to optimize the enhancement of two adjacent vibrational bands of a self-assembled thiol-monolayer. Varying the incident angle shifts the spectral positions at which collective excitation and peak field enhancement of the antennas occur. This allows a spectral tuning of the array resonance without changing geometry or surrounding material of the antennas.

Additionally, we now investigate the enhancement of vibrational modes of different numbers of CH_2-bonds by varying the chain lengths of the surface molecules.

[1] R.Adato et al., P. Natl. Acad. Sci. USA, **106**, 19227, 2009
[2] F.Neubrech et al., Phys. Rev. Lett, **101**, 157403, 2008
[3] T.W.W.Maß and T.Taubner, ACS Photonics, **2**, 1498, 2015

O 23.5 Mon 18:15 Poster E

Efficiency of Fano resonance in arrangements of nanorods: a comparison study — •Madeleine Nilsen[1], Manuel Gonçalves[1], Armen Melikyan[2], Hayk Minassian[3], Taron Makaryan[4], and Othmar Marti[1] — [1]Ulm University - Institute of Experimental Physics, Ulm, Germany — [2]Russian-Armenian (Slavonic) University, Yerevan, Armenia — [3]Yerevan Physics Institute, Yerevan, Armenia — [4]Drexel Nanomaterials Group, Drexel University, Philadelphia, USA

Nanorods allow easy tuning of optical resonances by varying the rod length and aspect ratio. Multipole resonances in rod-like nanoparticles are well separated and have relatively small bandwidths. Thus, assemblies of nanorods have been successfully used for generating Fano resonances.

In rods arranged in dolmen configuration, the dark mode necessary for the destructive interference of the Fano resonance is excited in both parallel rods simultaneously, with anti-symmetric surface charge density. In a H-like configuration of rods, quadrupole dark modes are excited independently in each long rods, resulting although in a mirror anti-symmetric surface charge density. Moreover, the near-field coupling of the H-like structure leads to a more pronounced Fano resonance than in the dolmen. H-like structures assembled in linear arrays with short separation comparing to the wavelength produce further attenuation of the scattering cross-section at the Fano dip.

The optical properties of the coupled nanorods were investigated by finite-element method (FEM). Nanorod structures were fabricated by e-beam lithography (EBL) and focused ion beam milling (FIB).

O 23.6 Mon 18:15 Poster E

Higher Harmonics Generation in Single Extended Gold Nanostructures — •Julian Obermeier, Thorsten Schumacher, Daniela Wolf, and Markus Lippitz — Experimental Physics III, University of Bayreuth

Higher harmonics generation in single gold nanostructures is a commonly known effect. Many fascinating experiments showed, that the nonlinear emission is strongly influenced and shaped by the particle plasmon resonance. However, when the structure dimension exceeds the diffraction limited excitation area, the higher order modes of the structure and even propagation of the fundamental and nonlinear field becomes important. In our experiments we investigate the spectrally dependent local nonlinear response of single gold nanostructures ranging from a few hundreds of nanometers to several micrometers in size. After excitation with pulsed infrared light, the locally generated second and third harmonic field is emitted in the near ultraviolet and visible spectrum and collected by a high NA oil immersion objective. This configuration allows a high spatial resolution of the origin of the nonlinear emission far below the diffraction limit of the excitation wavelength. In addition, the back focal plane pattern of the nonlinear emission carries information of its phase and directivity. On this poster, we present our method and first experimental results to determine the local emission properties of extended gold nanostructures.

O 23.7 Mon 18:15 Poster E

Ultrafast thermionic injection currents in metal-insulator-metal junctions — •Felix Becker[1], Detlef Diesing[2], Dominik Differt[1], Matthias Hensen[1], Walter Pfeiffer[1], and Christian Strüber[3] — [1]Molekül- und Oberflächenphysik, Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany — [2]Surface Dynamics Group, Fakultät für Chemie, Universität Duisburg-Essen, 45141 Essen, Germany — [3]Quantum Optics and Laser Science Research Group, Imperial College London, SW7 2AZ London, GB

Recently, it has been shown that plasmonic resonances at structural defects on the top electrode of the heterosystem facilitate the injection of charge carriers above the tunnel barrier of the oxide [1]. Here, we exploit the enhanced excitation in the vicinity of gold nanoparticle antennas deposited on the top electrode of a metal-insulator-metal junction to inject charge carriers in the counter electrode. Instead of multi-photon processes or strong field effects, we identify highly localized thermionic emission as the dominating process for current injection. Here the theoretical model describing the experimental observations is presented. It is based on the calculated electromagnetic field distribution, simulated excited electron relaxation cascades and solutions of the three-dimensional heat diffusion equation. The large temperature gradients in the electron gas and the corresponding ultrafast temperature transients give rise to highly localized and ultrafast thermionic injection currents. An injection current pulse duration of about 20 fs is obtained although the thermionic emission is dominating.

[1] D. Differt et al., Appl. Phys. Lett. 101, 111608 (2012)

O 23.8 Mon 18:15 Poster E

Femtosecond pump-probe transmission measurements of spatially inhomogenous electron heating caused by plasmonic excitation in gold gratings — •Jonas Vondran[1], Felix Spitzer[1], Ilya Akimov[1], Boris Glavin[2], Vladimir Belotelov[3], Sachin Kasture[4], Arvind S. Vengurlekar[4], Achanta V. Gopal[4], and Manfred Bayer[1] — [1]Technische Universität Dortmund, Dortmund, Germany — [2]V.E. Lashkaryov Institute of Semiconductor Physics, Kiev, Ukraine — [3]Lomonosov Moscow State University, Moscow, Russia — [4]Tata Institute of Fundamental Research, Mumbai, India

Periodically perforated gold films are subject to femtosecond resolved pump-probe transmission measurements which show ultrafast relaxation dynamics of optically excited electrons. Differential transmission is measured with varying incident angles and different polarisation configurations. Using biexponential fitting functions two distinct decay times can be observed in the transient data: A decay with a relaxation time of about 1 ps is attributed to electron-lattice energy transfer which is also present in unstructured gold films. A second, shorter relaxation is observed which shows a characteristic decay time of 200 to 300 fs. This decay is due to spatially inhomogeneous heat distribution inside the gold grating's slabs which causes an additional thermal diffusion process. Depending on the exciting pump polarisation this decay shows a changing sign which indicates an opposing direction of heat gradients with plasmonic compared to non-plasmonic excitation.

O 23.9 Mon 18:15 Poster E

Plasmonic metasurface enhanced non-linear optical effects in LiNbO3 optical waveguides — •Felicitas Walter[1], Andre Hildebrandt[2], Nils Weber[1], Jens Förstner[2], Cedric Meier[1], and Thomas Zentgraf[1] — [1]Department of Physics, University of Paderborn, Warburgerstr. 100, D-33098, Germany — [2]Department of Electrical Engineering, University of Paderborn, Warburger Str. 100, D-33098, Germany

In this project we exploring the possibilities to enhance the frequency conversion of light in LiNbO3 waveguides by utilizing plasmonic metasurfaces. In particular, we are investigating the effects of gold plasmonic nanoantennas arrays on Titanium undiffused Lithium Niobate (Ti:LiNbO3) waveguides. Two different kind of nanoanteannas were fabricated on top of the waveguides in a two-step electron-beam lithography and lift-off process. The metasurfaces are designed for a resonance wavelength of 1500 nm. As these antennas enhance the light field locally, they serve as an enhancement for nonlinear optical effects, e.g., second harmonic generation. To guaranty a phase matching as well as the coupling into the waveguide for light incident perpendicular to the surface, we tested various periodicities and arrangements of the antennas. Furthermore, an additional layer of TiO2 on top of the metasurfaces can further increase the coupling to the optical waveguide mode by lifting the mode profile more to the surface.

O 23.10 Mon 18:15 Poster E

strong coupling of surface plasmons and whispering gallery cavity — •qi ai, domenico paone, nikolai strohfeldt, simon ristok, and harald giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

A lot of research has focused on spectrally narrowing the plasmon resonance of metal nanoparticles, which could benefit the application of the localized surface plasmon resonance (LSPR) for sensing and nonlinear conversion. Here we demonstrate substantial reduction in the LSPR linewidth of an Au nanorod by depositing it onto the surface of a tapered fiber. When the taper diameter is reduced to about 1-3 μm, we observe signatures of strong coupling between the LSPR modes and the whispering gallery modes of the tapered fiber. This results in a very narrow hybrid plasmon-fiber resonance of the single Au nanorod, with a much higher quality factor (up to 300) when compared with that of an Au nanorod or an uncoated fiber with the same diameter. The strong coupling leads to a significant enhancement of the peak scattering intensity at plasmon resonance when compared to an uncoupled Au nanorod.

O 23.11 Mon 18:15 Poster E

Simulation of electric field patterns modified by metallic nanoantennas — •Richard Kerber, Doris E. Reiter, and Tilmann Kuhn — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

Metallic nanoantennas are known to greatly enhance light fields and the geometry of nanoantennas influences the polarization properties of the electric field. When a nanoantenna is coupled to a semiconductor nanostructure, e.g., a quantum dot, the polarization plays an important role in the creation of electron-hole pairs. Focussing on linear and circular polarization, we perform a systematic study of nanoantennas, revealing effects of geometry on the electric field polarization. For the simulation we use the boundary element method. We consider nanoantennas consisting of gold nanostripes, which are arranged in a circle around a gap region. Different geometries are studied by varying length and number of the stripes. The impact of symmetry in a dimer nanoantenna is analyzed by changing the angle between the two nanostripes. The results show a strong dependence of the electric field on the excitation polarization and the antenna geometry.

O 23.12 Mon 18:15 Poster E

Real-space imaging of nanotip plasmons using electron energy loss spectroscopy — •Benjamin Schröder[1], Thorsten Weber[2,3], Sergey V. Yalunin[1], Thomas Kiel[4], Christian Matyssek[4], Murat Sivis[1], Sascha Schäfer[1], Felix von Cube[2,3], Stephan Irsen[3], Kurt Busch[4,5], Sefan Linden[2], and Claus Ropers[1] — [1]4th Physical Institute - Solids and Nanostructures, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 12, 53115 Bonn — [3]Electron Microscopy and Analytics, center of advanced european studies and research, Ludwig-Erhard-

Allee 2, 53175 Bonn — [4]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin — [5]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin

Surface plasmon polaritons (SPPs) excited on the shaft of sharp metal tips provide electromagnetic field confinement and enhancement at the apex. Here, we study gold nanotips by scanning transmission electron microscopy combined with electron energy loss spectroscopy (STEM-EELS). Using this technique, we observe standing waves of plasmonic modes formed by SPP reflection at the tip apex. We provide a fully retarded model and numerical computations based on a discontinuous Galerkin time domain approach showing excellent agreement with the experimental data. Our results demonstrate a high reflectivity of the apex to the fundamental mode, with negligible contributions of higher order azimuthal SPP modes in the apex-near region[1].

[1] B. Schröder et al., Phys. Rev. B 92, 085411 (2015).

O 23.13 Mon 18:15 Poster E

Investigation of carrier concentrations in doped InAs using SNOM measurements to quantify and improve signal modelling — •Maximilian Sauer, Lena Jung, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

The scattering-type scanning near-field optical microscope (s-SNOM) consists of an AFM where the tip is illuminated by an infrared laser to create near-fields at the tips apex, which has a radius of typically 25nm. With SNOM it is possible to investigate the optical and electrical properties, including the dielectric function, of doped semiconductors with a spatial resolution that can be below the diffraction limit because it is given by the tip's radius. Hereby, the so called Finite Dipole Model (FDM) in combination with the Drude model is used to calculate SNOM signals to compare with actual measurement data. Within these models, the carrier concentration of a material can be extracted from the signals amplitude and phase at different wavelengths.

Doped bulk InAs samples with known electrical properties like carrier concentration due to investigation via other measurement techniques like Hall measurements are investigated with SNOM. The model's predictions based on our SNOM measurements can be compared with the known properties. The results of this comparison are used to examine if the models need to be improved in order to correctly describe the data. The next step is the expansion of the investigation to nanostructures, for example determining and imaging the electrial properties of nanowires, to make use of SNOM's high spatial resolution.

O 23.14 Mon 18:15 Poster E

Ideas on aSNOM using fiber optics — •Marco Klement, Jonas Albert, and Markus Lippitz — Universität Bayreuth, Bayreuth, Deutschland

Apertureless scanning near-field optical microscopy (aSNOM) is a tool to measure the electric fields of optical excitations on nano-particles with deep subwavelength resolution.

We will present our progress in implementing this method into an existing SNOM experiment and present ideas on how stability and signal to noise ratio could be improved using fiber optics instead of free space optics.

O 23.15 Mon 18:15 Poster E

Tip modified spectroscopy of nanowires — •Jonas Albert and Markus Lippitz — Universität Bayreuth

We are investigating 1D structures such as CdSe nanowires and wire-like molecular aggregates with an apertureless Scanning Near-field Optical Microscope (aSNOM). The optical fields at the near-field probe, a metal coated AFM-tip, are confined in a space much smaller than the wavelength and therefore showing a high field gradient on the nanometer scale. Utilising this near-field interaction we aim for modification of fluorescence emission by the presence of the near-field probe. Next to simple quenching we expect the optical field gradients to enhance dipole forbidden higher-order transitions.

O 23.16 Mon 18:15 Poster E

Long-lived coherence in the metal-organic hybrid Cobalt/Alq3 — Martin Aeschlimann[1], Tobias Brixner[2], Mirko Cinchetti[1], Norman Haag[1], Matthias Hensen[3], •Bernhard Huber[2], Christian Kramer[2], Walter Pfeiffer[3], Martin Piecuch[1], Christian Schneider[1], Benjamin Stadtmüller[1], and Philip Thielen[1] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

The coherent electron dynamics of optically pumped (400 nm) molecular states of the metal-organic complex tris(8-hydroxyquinolinato)aluminium (Alq3) deposited on Cobalt are investigated with time-resolved photoemission microscopy (PEEM). We observe a coherence signal in interferometric autocorrelation traces when probing the excited-state manifold of Alq3 with 800 nm laser pulses. In two-dimensional (2D) nanoscopy spectra, two excited states are identified with an energy spacing of about 77 meV with respective linewidths of 11 meV and 48 meV. Measuring the kinetic energy of the photoelectrons, these features prevail over the entire accessible energy range of about 1 eV. The observed signal can be explained by long-lived coherent excited states of the adsorbate that decay among others via coupling to excited electrons in the substrate giving rise to a photoemission signal that depends linearly on the laser intensity.

O 23.17 Mon 18:15 Poster E

Fine-tuning and individual addressing of mid-IR nanoantenna resonances by reversible optical switching of Ge3Sb2Te6 thin-films — •Ann-Katrin U. Michel, Dmitry N. Chigrin, Thomas Kalix, Angela De Rose, Matthias Wuttig, and Thomas Taubner — RWTH Aachen University, 1. Institute of Physics A, Otto-Blumenthal-Straße, 52074 Aachen

Metallic nanostructures with well-defined resonances are a key building block for nanoscale photonic ”meta-devices”. The post-fabrication control over the nanostructures resonances is fundamental for enabling reconfigurable devices based on metamaterials, which allow for all-optical switchable nanophotonic imaging and sensors [1].

We present the tuning of the spectral position of the nanostructure resonance frequency by locally addressing phase-change material (PCM) thin-films with single nanosecond laser pulses. PCMs offer a huge contrast in the refractive index n due to a phase transition from their amorphous to their crystalline state. By optically induced local phase transitions, the effective n of the PCM medium, which affects the resonant structures resonance, can be tuned over a broad range.

The variation of the PCM area switched by a laser pulse allows us to reversibly alter the nanostructure resonance frequency of a 600 nm long rod-shaped antenna stepwise in the mid-infrared spectral range [2]. The local addressing enables a multi-step tuning of single nanostructures pointing towards actively controllable metasurfaces.

[1] Zheludev, N. I. et al. Nat. Mater. 11 (2012).

[2] Michel, A. U. et al. in preparation

O 23.18 Mon 18:15 Poster E

Single Molecule Spectroscopy in a tunable cavity system — •Oliver Schneider[1], Ulrich Müller[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius-Maximilian-Universität, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Organic molecules are suitable quantum systems for single photon sources (SPS) as their high exciton binding energies allow for room temperature operation in contrast to inorganic semiconductors [1].

For the implementation of an electrically driven SPS, control of the triplet lifetime is desirable. Drexhage [2] already showed how ensemble lifetimes can be tuned with varying the distance between quantum emitters and a metallic surface. This type of experiment has been advanced for single molecules by using piezo controlled mirrors [3].

Here we report on a novel approach for electrically tuning the molecule-mirror distance by means of an Al-covered support embedded directly within the sample layout. As demonstrated by interferometric measurements, a displacement of about 70 nm, corresponding to about $^{\lambda}/_{4}$, is feasible by this arrangement.

Measuring photon statistics on selected single molecules while simultaneously varying the distance to the reflecting Al-interface, we demonstrate the voltage-driven control of radiative lifetimes of individual quantum emitters located within the device.

[1] M. Nothaft et al., *Nature Comm.* **3**, 628 (2012)

[2] K. H. Drexhage, *Prog. Opt.* **12**, 165 (1974)

[3] B. C. Buchler et al., *Phys. Rev. Lett.* **95**, 063003 (2005)

O 23.19 Mon 18:15 Poster E

Coherent energy transfer between widely separated nanoantennas coupled via an elliptic cavity — Martin Aeschlimann[1], Tobias Brixner[2], •Benjamin Frisch[1], Bert Hecht[3], Bernhard Huber[2], Matthias Hensen[4], Christian Kramer[2], Enno Krauss[3], Thomas Löber[5], Walter Pfeiffer[4], Martin Piecuch[1], and Philip Thielen[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Department of Physical and Theoretical Chemistry, Würzburg University, 97074 Würzburg, Germany — [3]Experimental Physics 5, Würzburg University, 97074 Würzburg, Germany — [4]Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [5]Nano-Structuring-Centre, TU Kaiserslautern, 67663 Kaiserslautern, Germany

We present experimental and theoretical results on a system that allows long-distance coupling between two plasmonic nanoantennas mediated by an extended SPP mode in an elliptic cavity. The system is the first to demonstrate a prearranged hybridization of two seperated LSPs and a propagating surface plasmon. It is prepared on atomically flat single crystalline gold flakes and temporal dynamics of plasmonic excitations are investigated by time-resolved photoelectron emission microscopy (PEEM). The observed coherent back and forth transfer of energy between the nanoantennas is well explained by a model of three coupled oscillators. Spectrally-resolved PEEM experiments support the demonstration of hybridization.

O 23.20 Mon 18:15 Poster E

Tuning the plasmon-exciton resonance of Gold-TDBC core-shell particles via the surrounding medium — •Felix Stete[1,2], Wouter Koopman[1], and Matias Bargheer[1,3] — [1]Universität Potsdam, Institut für Physik und Astronomie, 14476 Potsdam, Germany — [2]Humboldt-Universität zu Berlin, School of Analytical Sciences Adlershof (SALSA), 10099 Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Wilhelm-Conrad-Röntgen Campus, BESSY II, 12489 Berlin, Germany

We present a method to tune the resonance frequencies of a plasmon-exciton system leading to an anti-crossing of the resonance peaks. The investigated plasmon-exciton system is given by gold nanospheres coated with the cyanine dye TDBC. The surrounding medium is gradually changed by a layer-by-layer deposition of polyelectrolytes with alternating charge forming well-defined double layers. We explain the dependence of the core-shell particles' spectrum on the surrounding medium by the shift of the uncoupled plasmon resonance given by the effective dielectric function of the composite particle-air-polyelectrolyte medium. The uncoupled exciton resonance is approximately unchanged by the changing environment. The strong coupling characteristics of the plasmon-exciton system are demonstrated by an anti-crossing behaviour of the resonance peaks.

O 23.21 Mon 18:15 Poster E

Radiation patterns of semiconductor nanocrystals coupled to optical dimer antennas — •Nicolas Coca Lopez[1], Annick Hemmerling[1], Harald Budde[1], Francesca Nicoli[2], Tao Zhang[2], Mauricio Pilo-Pais[2], Tim Liedl[2], and Achim Hartschuh[1] — [1]Department of Chemistry, and Center for NanoScience (CeNS), LMU München, Germany — [2]Department of Physics, and Center for NanoScience (CeNS), LMU München, Germany

Optical antennas can be used to manipulate the coupling between emitters and the radiation field leading to changes in the rate and direction of spontaneous emission [1,2]. Here we study single semiconductor nanocrystals (NC) enclosed at the feed-point of plasmonic dimer antennas formed by DNA-based self-assembly [3]. Radiation patterns recorded by back-focal plane (BFP) imaging of the photoluminescence (PL) emission of single NC-antenna systems show the antenna directivity and the spontaneous emission rate enhancement. Quantitative model calculations of the BFP patterns are carried out to determine the coupling strength of the different transition dipole moment orientations in the NC to the antenna resonance.

[1] Bharadwaj, P. et al., Adv. Opt. Photon. 1, 438 - 483, (2009).
[2] Curto, A. G. et al., Science 329, 930 - 933, (2010).
[3] Kuzyk, A. et al., Nature 483, 311 - 314, (2012).

O 23.22 Mon 18:15 Poster E

Electrodynamics of Gold Nano-Sponges — •Felix Schwarz, David Leipold, and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, TU Ilmenau

Taylored disorder can prove most beneficial in nanophotonics: Not only are systems inherently unaffected by perturbations caused by, e.g., temperature, but also disorder-induced localization can appear and symmetry-breaking causes light-trapping in otherwise dark modes. Recently, irregular nanoporous gold sponges with a diameter of around 200nm and features on the 20nm scale made by clever metallurgy were presented [1]. Our numeric calculations of plasmonic resonances show that surprisingly long-lived modes with greatly enhanced near-field intensities can be excited. The results reproduce important aspects of scattering and nonlinear photoemission spectra found in recent experimental studies [1,2]. These are intuitively explained in terms of interacting near-field modes and their coupling to the far-field. Furthermore, we discuss the impact of our findings on future practical applications, e.g. in chemical sensing.

[1] C. Vidal et al., ACS Photonics, 2, 1436 (2015)
[2] G. Hegert, C. Lienau, private communication

O 24: Plasmonics and Nanooptics: Fabrication, Characterization and Applications

Time: Monday 18:15–20:30 Location: Poster E

O 24.1 Mon 18:15 Poster E

Resonant energy-transfer in plasmonic hybrid arrays — •Julian Sindram, Joseph P. S. Fitzgerald, and Matthias Karg — Physical Chemistry I, University of Bayreuth, Bayreuth, Germany

Energy transfer between plasmonic nanoparticles (NPs) and fluorophores drastically alter the spectral response of the involved species and can be harnessed to create plasmonic nanolasers. Such lasers can be nanoscopic sources of coherent light with high potential for many applications in the field of nano-optics. Energy transfer rates depend on various parameters, including the NP material and size, the optical properties of the fluorophore, the distance between NPs and fluorophores and the concentration of fluorophores. In order to achieve a better understanding of energy transfer processes, a screening of numerous parameter combinations is necessary.

We present a new and efficient approach, allowing us to prepare and analyze large parameter sets on a single substrate. A bottom-up preparation procedure is used to fabricate substrate supported silver NP arrays with a spatial gradient of particle sizes. These plasmonic arrays are embedded in a fluorophore host matrix. Position-dependent steady-state and time resolved fluorescence spectroscopy, as well as extinction spectroscopy, are employed to examine energy transfer.

O 24.2 Mon 18:15 Poster E

Macrocopic self-assembled anisotropic metal-insulator-metal nanoparticles for tunable magnetic modes — •Max Schnepf[1], Martin Mayer[1], Moritz Tebbe[2], Tobias A.F. König[1], and Andreas Fery[1] — [1]Leibniz Institute of Polymer Research (IPF), Institute of Physical Chemistry and Polymer Physics, Hohe Str. 6, 01069 Dresden — [2]Dept. of Physical Chemistry II, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth

We present the synthesis and optical characterization of anisotropic metal-insulator-metal nanoparticles featuring intrinsic metamaterial properties within the visible wavelength range. The nanoparticle consists of a single crystalline gold nanorod core and a silver/gold hybrid nanobox shell, separated by a dielectric spacer. The magnetic mode can be tailored by distance variations between the nanorod core and the nanobox using a three-step synthesis. To clearly distinguish between the longitudinal and transversal mode, we have incorporated the anisotropic nanoparticle into a stretchable polymer film (polyvinyl alcohol, PVA). Stretching of the polymer film results in macroscopic alignment of the nanoparticles. Using conventional UV/vis scattering and absorption spectroscopy, we were able to identify the absorption dominated magnetic modes. We confirmed the magnetic mode properties with finite-difference time-domain (FDTD) simulations. This simple and rational particle design is capable of enabling bottom-up fabrication of colloidal optical metamaterials on macroscopic areas.

O 24.3 Mon 18:15 Poster E

Coupling of quantum well emission to surface plasmon modes in rolled-up microtubes — •Jan Siebels, Hoan Vu, Tobias Kipp, and Alf Mews — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

It has recently been shown that dielectric grating structures with gradually varying effective refractive indices in the direction perpendicular to the periodicity can be utilized for the excitation of surface plasmons in a wide spectral range [1]. This general idea of broad band surface plasmon excitation can be transferred to simple metallic gratings with gradually varying filling-factors. Here, we present the fabrication and optical characterization of silver grating structures positioned in rolled-up microtubes with embedded quantum well heterostructures. Spectrally- and time-resolved photoluminescence spectroscopy shows spectral shifts and changes of the decay lifetime exclusively in those areas of these structures in which calculations indicate an overlap between surface plasmon dispersion and emission energy of the quantum well. Based on these observations we propose and discuss possible coupling mechanisms.

[1] J. Ehlermann et al., Appl. Phys. Lett. 106, 101106 (2015).

O 24.4 Mon 18:15 Poster E

Automatized Optical Switching of Phase Change Material for Mid - Infrared Resonant Structures — •Julian A. Hanss, Martin Lewin, Tobias W.W. Mass, and Thomas Taubner — Institute of Physics (IA) RWTH Aachen

Confinement and local enhancement of electric fields can be achieved by metallic resonant structures. Dimensions and optical properties of the structure and surroundings define the position and strength of the resonance. Optical or thermal switching between different metastable phases of Phase Change Materials (PCMs) with distinct optical properties provide the opportunity of reversible, post - fabrication tuning of such resonances [1]. Focused laser beams change the structural phase of the PCM on a microscale, providing the possibility to switch for example single antennas of an array or write arbitrary structured optical metasurfaces [2].
By automatizing a previously built laser setup, the efficiency of structure modulation is increased facilitating fast investigations of different structures and material combinations. Localized, reversible tuning of resonant structures and and writing of arbitrary patterns can be achieved to create predefined optical responses.

[1] A. Michel et al., Nano Lett., 13(8), pp 3470-3475 (2013)
[2] Q. Wang et al., arXiv: 1508.03818 [physics.optics]

O 24.5 Mon 18:15 Poster E

Plasmonic gradient structures: Nanorod arrays with high spectral tunability — •Matthias Böhm[1], Susan Derenko[1], Vera Fiehler[1], Fabian Patrovsky[1], Stephan Barth[2], Hagen Bartzsch[2], Peter Frach[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Deutschland — [2]Fraunhofer-Institut für Organische Elektronik, Elektronenstrahl- und Plasmatechnik Dresden (FEP), 01277 Dresden, Deutschland

Nanorod arrays are fabricated for instance by anodizing aluminum thin films with acidic solutions such as sulfuric acid or oxalic acid [1]. When altering the anodization conditions, different pore sizes and inter-pore distances are achieved, hence leading to plasmonic nanorod arrays that offer a broad range of spectral tunability when filling the pores with e.g. gold or silver. It is well known that the plasmonic resonance properties strongly depend on the aspect ratio (length-to-diameter) of individual particle antennas [2]. However, when fabricating antenna arrays, the distance between adjacent rods becomes crucial and thus needs to be controlled by the fabrication method and conditions.

Our study here presents a experimental and theoretical analysis of how the geometrical parameters must be varied in order to achieve antenna gradient structures within one sample that allows spectral tunability over several hundred nanometers in the optical wavelength range.

[1] M. Wang, Y. Liu, and H. Yang, Electrochim. Acta 62, 424 (2012).
[2] S.W. Prescott and P. Mulvaney, J. Appl. Phys. 99, 123504 (2006).

O 24.6 Mon 18:15 Poster E

Controlled growth of high aspect-ratio single-crystalline gold-platelets — •Enno Krauss[1], René Kullock[1], Guilherme Stein[1], Peter Geisler[1], and Bert Hecht[1,2] — [1]NanoOptics & Biophotonics Group, Experimentelle Physik 5, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Röntgen Research Center for Complex Material Systems (RCCM), Am Hubland, 97074 Würzburg, Germany

Advances in nano-fabrication increase the need for high-quality single-crystalline gold-substrates that combine large areas to enable lithographic methods with low and tunable thickness. We present a simple recipe to chemically grow high quality single-crystalline gold-platelets with thicknesses of less than 20 *nm* combined with edge lengths up to 0.2 *mm*. The reactants are tuned and their impact on the growth-velocities of height and lateral size is statistically investigated. By varying the chemical environment during growth, the thickness can be tuned independently of the lateral size.

O 24.7 Mon 18:15 Poster E

Construction of a tip-enhanced Raman spectroscopy system and gold tip fabrication — •Marcel Weinhold[1], Thomas Sander[1], Jalmar Tschakert[2], Thomas Göddenhenrich[2], André Schirmeisen[2], Sangam Chatterjee[1], and Peter J. Klar[1] — [1]Justus-Liebig-Universität Gießen, I. Physikalisches Institut, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, 35392 Gießen

Raman spectroscopy is a powerful technique for analyzing molecular vibrations as well as lattice dynamics in bulk materials. However, Raman signals are of an weak intensity and the scattering volume probed is rather large, roughly about (500 nm)^3. Metallic Scanning Probe Microscope (SPM) tips acting as nanoantennas enhance the signal in a small area (hot-spot) by several orders of magnitude. The phenomenon is known as tip-enhanced Raman spectroscopy (TERS). Due to the fact that reliable tip preparation is still challenging, we fabricated suitable tips by etching a gold wire, sputtering a thin layer of gold on standard Si AFM-tips, and by using an Au e-beam resist. These tips were analyzed with respect to surface roughness, apex radius, and enhancement factor. The latter investigations were carried out on the TERS-system constructed by us and compared with studies on a commercially available one.

O 24.8 Mon 18:15 Poster E

Surface potential studies on nanostructured plasmonic films under monochromatic illumination — •Ömer Akay[1], Eser M. Akinoglu[1,2], Klaus Schwarzburg[3], and Michael Giersig[1,3] — [1]Freie Universität Berlin, Department of Physics, Berlin, Germany — [2]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam-Golm Science Park, Potsdam, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut Nanoarchitekturen für die Energieumwandlung, Berlin, Germany

Recently, surface potential changes were observed when plasmon active and optically thin metal films with periodic perforations on the nanoscale are illuminated with monochromatic light in the range of the plasmon resonance of the studied nanostructured film. This effect is described as a plasmoelectric effect that could convert optical energy into electrical potential differences in absence of semiconductors. An applied fabrication method to obtain plasmon active nanostructured metallic films with hexagonally ordered perforations is nanosphere lithography (NSL) in conjunction with plasma etching and physical vapour deposition. We present the characterisation of our systems with optical spectroscopy, atomic force microscopy (AFM) and we study the impact of monochromatic light on plasmon active optically thin and nanostructured metallic films via surface potential measurements using Kelvin probe force microscopy (KPFM) under simultaneous illumination in the energy range of the plasmon resonance peak of our system towards observing plasmoelectric effects.

O 24.9 Mon 18:15 Poster E

Plasmonically enhanced perovskite solar cells for photovoltaics — •Jonas Schwenzer[1], Domenico Paone[1], Justus Back[2], Sabine Ludwigs[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCOPE, University of Stuttgart, Germany — [2]Institut für Polymerchemie, Universität Stuttgart, Germany

Perovskite solar cells are the most promising alternative to silicon solar cells. Their record efficiency has increased from 9% to over 20% within the last three years. Further improvements are only possible if the photon to electron conversion efficiency can be increased. Here, we incorporated gold nanoparticles into the alumina scaffolding layer of perovskite solar cells to excite localized surface plasmon resonances. We investigated the short circuit current, open circuit voltage, external quantum efficiency, and power conversion efficiency in dependence of the gold nanoparticle concentration. A decrease in voltage was compensated by an increased current for optical densities below 0.1. Hence, the efficiency could be increased by 53% and 32% for optical densities of 0.05 and 0.1, respectively. Higher nanoparticle concentrations lead to decreased voltages and currents. Thus, we conclude that low concentrations of gold nanoparticles can be used to increase the current and thereby the performance of perovskite solar cells.

O 24.10 Mon 18:15 Poster E

Nonlinear holography using plasmonic metasurfaces — •Bernhard Reineke[1], Guixin Li[2], Shumei Chen[2], Franziska Zeuner[1], Nitipat Pholchai[3], Polis Wing Han Wong[4], Edwin Yue Bun Pun[4], Kok Wai Cheah[2], Shuang Zhang[2], and Thomas Zentgraf[1] — [1]Department of Physics, University of Paderborn, Warburger Straße 100, 33098 Paderborn — [2]School of Physics and Astronomy, University of Birmingham, Birmingham B15 2TT, UK — [3]Department of Industrial Physics and Medical Instrumentation, King Mongkuts University of Technology North Bangkok, 1518 Pibulsongkram Road, Bangkok 10800, Thailand — [4]Department of Electronic Engineering, City University of Hong Kong, 83 Tat Chee Avenue, Hong Kong

Recently it was shown that high-resolution holograms can be realized by using plasmonic metasurfaces. Combining nonlinear metasurfaces and holography can lead to new highly unconventional and versatile optical devices.

Here, we show a way to generate nonlinear holograms in the visible spectral range by using Second Harmonic Generation. For this purpose we fabricated a plasmonic nonlinear metasurface consisting of plasmonic nanoantennas. The desired phase for the hologram is hereby encoded in the arrangement and orientation of the antennas. By imaging the nonlinear second harmonic signal from the sample when illuminated with RCP or LCP short laser pulses we can reconstruct the image. Furthermore, we demonstrate that multiplexing of holographic images can be obtained.

O 24.11 Mon 18:15 Poster E

Large-area olasmonic devices for hydrogen sensing — •Ramon Walter, Nikolai Strohfeldt, Florian Sterl, Jonas Schwenzer, and Harald Giessen — 4th Phsics Institute and Research Center SCOPE, University of Stuttgart

Hydrogen has the potential to be a source of clean energy when used in fuel cells. However, it also poses potential hazards. A sensitive and reliable sensor can reduce this risk. Plasmonics can serve as an ideal building block for such sensor devices. By changing the optical properties of such a device under hydrogen exposure, the plasmon resonance shifts depending to the amount of hydrogen.

An ideal plasmonic material is gold. Due to the fact that gold nanoparticles are not reacting to hydrogen, it is necessary to cover these particles with a dielectric film consisting of hydrogen sensitive and transparent films, like Titaniumdioxide and zinc oxide.

We present the feasibility of such devices, using TiO2. By using a combination of directional argon-ion-beam-etching and colloidal lithography we produce gold nanodisks on a large-area scale. By spincoating we deposit a thin film of TiO2 on top and finally add a thin palladium catalyst layer. The resulting device shows a well modulated resonance with low transmission. By changing from pure nitrogen atmosphere to a hydrogen content of 5 %, the resonance shifts to longer wavelengths and the transmission increases.

The sensitivity of our design can optimized by tailoring thickness of the dielectric layer, leading to industrially viably hydrogen sensor coatings for a multitude of practical applications.

O 25: Oxide and Insulator Surfaces: Structure and Growth

Time: Monday 18:15–20:30 Location: Poster E

O 25.1 Mon 18:15 Poster E

Oxidation of epitaxial iron films on Ag(001) — •Jari Rodewald, Daniel Bruns, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

Ferrimagnetic magnetite Fe_3O_4 with inverse spinel structure is a promising candidate for magnetic devices like giant magneto resistance (GMR) and tunneling magneto resistance (TMR). In order to develop these devices and to select certain iron oxide phases it is important to understand the structure and growth properties of such oxide films.
Hence, this work investigates the oxidation process of crystalline iron films with respect to different annealing temperatures and oxygen pressures. Therefore, pure bcc-iron is deposited on Ag(001) substrates by molecular beam epitaxy (MBE) and the oxidation process is divided into three consecutive steps of pre-annealing, UHV-annealing and post-annealing.
Surface structure and morphology are analyzed by spot profile analysis low energy electron diffraction (SPA-LEED), while the chemical composition of the surface is investigated by Auger electron spectroscopy (AES). Additionally, grazing incidence x-ray diffraction (GIXRD) measurements are performed in order to obtain information on the bulk structure of the deposited films.
The largest amount of magnetite is generated by post-annealing at 400°C and an oxygen pressure of $1 \cdot 10^{-5}$ mbar, while higher temperatures reduce the amount of oxygen and induce a structural change at the surface.

O 25.2 Mon 18:15 Poster E

Oxygen-induced phase switch of sub-monolayer iron oxide on Ir(100) — •Christopher Sobel, Pascal Ferstl, Lutz Hammer, and M.Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

By means of STM and LEED we show that two different sub-monolayer iron oxide phases exist on the Ir(100) surface which can be converted into each other by changing the chemical potential of oxygen. In oxygen poor conditions a 3×1-phase of one-dimensional FeO_2 wires forms which covers the whole surface homogeneously. In contrast oxygen rich conditions lead to a condensation into compact islands of quasi-hexagonal FeO(111) with an incommensurate "c(8.8×2)"-structure. The remaining iridium surface is covered by a pure oxygen 2×1-O phase [1]. The energy gain when forming the latter appears to be the driving force for the switch between the extended 3×1 and the compact island iron oxide phase. The behaviour differs qualitatively from other transition metals as for example cobalt, where in oxygen rich conditions the wires change from CoO_2 to CoO_3 stoichiometry. This fact indicates a delicate energy balance between the different phases.

[1] K. Johnson *et al.*, J. Chem. Phys. **112**, 10460 (2000)

O 25.3 Mon 18:15 Poster E

***Ab initio* Raman-spectroscopic study on Ce-Zr-Oxides** — •Marcel Giar, Michael Bachmann, Limei Chen, Peter J. Klar, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

Mixed Zr-Ce-oxides may serve as oxygen-storing co-catalysts in automotive applications or as catalytically active species in oxidation reactions. Amongst these, κ-$Ce_2Zr_2O_8$ is particularly known for its excellent oxygen storage capacity (OSC). This phase may be obtained from the so-called pyrochlore phase *pyr*-$Ce_2Zr_2O_7$ by incorporating oxygen, thereby oxidizing Ce^{3+} to Ce^{4+}. The underlying structural transition form the pyrochlore to the κ-phase is the key to understanding the superb OSC. Being very sensitive to structural differences, Raman spectroscopy is a well-suited method for investigating differences between crystal phases on a structural, electronic and vibrational level. Hence, in order to understand structural as well as electronic differences of both phases we calculate Raman susceptibilities and derived spectra based on DFT calculations. With our theoretical results we aim to interpret experimental Raman spectra.

O 25.4 Mon 18:15 Poster E

Complex dielectric function of $SrTiO_3$ and $BaTiO_3$ by HREELS — •Florian Schumann[1], Klaus Meinel[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle

Phonons and their softening are key elements for the phase transitions in ferroelectrics and multiferroics. In thin films, the phonons depend sensitively as well as the phase transition temperatures on the strain within the film. Here we report on high-resolution electron energy loss spectroscopy (HREELS) on the (001) and (111) surfaces of $BaTiO_3$ and $SrTiO_3$. HREELS reveals three dipole-active phonon polaritons, which are derived from the known transversal optical bulk phonons. In addition, it will be demonstrated that the complex dielectric function in the energy range from 4 to 1000 meV can be quantitatively extracted from the experimental loss function. This opens up the additional characterization of oxide doping levels as will be discussed for single crystal surfaces and thin films down to one unit cell thickness.

O 25.5 Mon 18:15 Poster E

Structural and magneto-optic properties of epitaxial iron films on MgO(001) — •Jannis Thien[1], Olga Kuschel[1], Timo Oberbiermann[2], Timo Kuschel[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [2]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

For years it is known that the linear magneto-optic Kerr effect depends on the wavelength of the applied laser. The currently outstanding question is a wavelength dependence for the quadratic magneto-optic Kerr effect as proposed by theoretical calculations for cubic crystals [1]. In order to compare the theoretical predictions with experiment, crystalline samples are needed. Thus, epitaxial iron films were grown by molecular beam epitaxy on MgO(001) at different temperatures. Each sample was capped with an amorphous silicon film at room temperature to prevent oxidation of the iron film. For the purpose of examining the purity of the evaporated iron, XPS measurements were made. The structural characterization was realised by LEED, XRR, AFM and XRD measurements. The magnetic properties were probed by MOKE experiments. Both chemical composition and structural as well as magnetic properties of the iron film change with increasing deposition temperature. From these results the sample with the most promising characteristics was choosen for the study of wavelength dependence of the quadratic magneto-optic Kerr effect.

[1] Hamrlová et al., submitted

O 25.6 Mon 18:15 Poster E

A first step of twin polymerization to study: The self-assembly of the twin monomer Spiro at the LSI influenced by sonication and deposition substrate temperature. — •Yen D.C Nguyen[1], Ha N.T Nguyen[1], Michael Hietshold[1], Thomas Ebert[2], and Stefan Spange[2] — [1]TU-Chemnitz, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — [2]Polymer Chemistry Group, Institute of Chemistry, TU-Chemnitz

The twin monomer 2,2*-spirobi [4H-1,3,2-benzo-dioxasiline] (SBS) consisting of building blocks bonded together covalently has been used to produce organic*inorganic nanostructured hybrid materials. The polymerization is initiated by ring opening of the 4H-1,3,2- benzodioxasilines or cleavage of the Si-O-C bonds. This way generates two structurally different homopolymers (silicon dioxide and a phenolic resin). Self-assembly of this twin monomer (SBS) at undecanol/HOPG interface investigated by STM at the liquid-solid interface (LSI) influenced by sonication and deposition substrate temperature. Firstly, by sonicating SBS/undecanol solution samples in different time periods the polymerization of spiro monomer at undecanol/HOPG has been observed without any catalyst. Secondly, the polymerization of spiro monomer can also be controlled by the substrate temperature during the deposition of the molecules out of the solution. By increasing the temperature of the pre-heated substrate, various periodic assemblies of spiro (dimer, trimer or pentamer resin) can be obtained.

O 26: Oxides and Insulator Surfaces: Adsorption

Time: Monday 18:15–20:30 Location: Poster E

O 26.1 Mon 18:15 Poster E

Vibrational Spectroscopic Studies of Formaldehyde Adsorption on Rutile TiO_2(110) — •Xiaojuan Yu[1], Chengwu Yang[1], Fabian Bebensee[1], Alexei Nefedov[1], Zhenrong Zhang[2], Qingfeng Ge[3], Zdenek Dohnálek[4], Yuemin Wang[1], and Christof Wöll[1] — [1]Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344 Karlsruhe, Germany — [2]Department of Physics, Baylor University, Waco, Texas 76798, USA — [3]Department of Chemistry and Biochemistry, Southern Illinois University, Carbondale, Illinois 62901, USA — [4]Institute for Interfacial Catalysis, Pacific Northwest National Laboratory, Richland, Washington 99352, USA

TiO_2 is one of the most important metal oxides used in catalysis and photocatalysis. The interaction of TiO_2 with aldehydes is of particular interest due to its promising applications in ethanol fuel cells, hydrogen production, biomass and in the control of air pollution. Here, the adsorption of formaldehyde (CH_2O) on the rutile TiO_2(110) surface was studied by infrared reflection-absorption spectroscopy (IRRAS). The IR data reveal the presence of different species depending on the temperature and coverage. The CH_2O monomer is identified after submonolayer adsorption at 70 K, in which CH_2O is weakly bound to the surface Ti_{5c} sites. Further adsorption at 70 K leads to the formation of multilayer CH_2O, which desorbs completely upon heating to 120 K. Simultaneously, paraformaldehyde is formed at Ti_{5c} sites along [001] direction and becomes the dominant surface species. In addition, dioxymethylene is detected as a minority one formed via reaction of CH_2O with neighboring O_{br} along [1-10] direction.

O 26.2 Mon 18:15 Poster E

Dimerization of benzoic acid on TiO_2 surfaces—an ab-initio study — •Wolfgang Heckel, Tim Würger, and Stefan Müller — Hamburg University of Technology, Institute of Advanced Ceramics

At the hybrid organic–metal-oxide interface intermolecular forces may contribute to improving mechanical stability. For instance linker molecules possessing an aromatic side chain interact with each other via van-der-Waals interaction.

In this regard, the adsorption of benzoic acids on TiO_2 (110) rutile serves as a prototype system. A very regular 2 × 2 overlayer due to dimerization via the phenyl groups has recently been reported [1].

Here, we present a density functional theory analysis of the dimerization of benzoic acids on both, anatase and rutile TiO_2 surfaces. To properly describe the attractive interaction of adsorbing molecules among each other, we applied an exchange correlation functional with van-der-Waals correction. For all surface orientations, the prefered dimer formation mode (hydrogen–to–π-orbital or tilted and twisted π–to–π) as well as the amount of energy gain resulting from dimerization will be discussed.

[1] Grinter et al., J. Phys. Chem. Lett. **5**, 4265 (2014).

Supported by DFG, SFB 986, project A4.

O 26.3 Mon 18:15 Poster E

Coverage-dependent behaviour of water on hematite(0001) from first principles — •Roman Ovcharenko and Elena Voloshina — Humbold-Universität zu Berlin, Berlin, Germany

It is well established that the water adsorption behaviour at high coverage regime may differ drastically from its adsorption at low coverage. The hydrogen bond network between polar water molecules and their residues tends to stabilize the water layer structure on top of a surface preventing following dissociation. Thus, the qualitative changes from the dissociative adsorption to the molecular one were found to take place on top of the aluminium oxide (0001) surface, which is isomorphic to hematite, at coverage more than 1 ML. For magnetite(001) such mixed dissociative-molecular adsorption was established already for the second water molecule in the 2x2 unit cell. Partially inheriting the properties of both aforementioned metal oxides, the hematite surface may affect the upper water layers forcing them to demonstrate adsorption behaviour different to the one on aluminium oxide or magnetite.

Here we present the theoretical study of the water adsorption on top of the hematite(0001) single-iron termination within the PBE+U+D level of accuracy to account for both the Fe 3d strongly correlated electrons as well as the weak dispersion interactions between water fragments on top of the surface.

O 26.4 Mon 18:15 Poster E

In-situ studies on the growth and functionalization of

MgO/Ag(100) — •Sabrina Pechmann[1], Gina Peschel[2], Hagen Klemm[2], Thomas Schmidt[2], and Rainer Fink[1] — [1]Physical Chemistry, FAU Erlangen-Nuremberg, Erlangen, Germany — [2]Chemical Physics, Fritz-Haber-Institute of the Max Planck Society, Berlin, Germany

Metal oxide thin films on metal supports are important for various technological applications like catalysis or the fabrication of electronic devices [1]. Surface modification and functionalization plays an important role to tune the oxide surface properties. We investigated the in-situ growth and structural properties of epitaxial MgO thin films on Ag(100) using surface-sensitive LEEM and XPEEM. MgO on Ag(100) serves as an attractive model system as the lattice mismatch between both bulk structures is only 3.1%, allowing epitaxial growth with just a small number of grain boundaries [2]. MgO is sensitive to both, electron and x-ray illumination. We could follow the structural modifications. While electrons induce a long-range ordered superstructure different from the pristine material, x-ray illumination induces the formation of square-like nanostructures. We attribute the long-range order to H2O or OH adsorption, which has been further investigated by temperature-programmed desorption (TPD). The adsorption of medium-sized organic molecules on thus modified surfaces will be compared to the non-reconstructed surfaces. This work is funded by the DFG within the funCOS research unit (FOR 1878) [1]Kramer, J. et al., Surf. Sci. 517, 87-97, 2002 [2]Valeri, S. et al., Surf. Sci. 507-510, 311-317, 2002

O 26.5 Mon 18:15 Poster E

Self-assembly of polycyclic aromatic hydrocarbons on bulk MgO(001) — •Tim Sander[1], Maximilian Ammon[1], Natalie Hammer[2], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, FAU Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg, Germany

MgO is a wide band gap insulator and a prototype oxide material with interesting catalytic properties. First, we report on the surface preparation and characterization of clean MgO(001) surfaces based on atomically resolved non-contact atomic force microscopy (nc-AFM) measurements. The MgO surfaces were cleaved in ultra-high vacuum using a home-built cleaving device and annealed prior to imaging to compensate surface charges. Second, we discuss the self-assembly of halogen-substituted bridged triphenylamine derivatives on MgO(001). Molecularly resolved nc-AFM images were performed to analyze the adsorption geometry and sites of the molecules.

O 26.6 Mon 18:15 Poster E

LEED-FTIR-DFT investigation of a twodimensional mixed phase $CO_2\cdot C_2H_2$ adsorbed on the KCl(100) surface — •Jochen Vogt — Uni Magdeburg, Magdeburg, Germany

Results from aerosol chemistry point towards the existence of a mixed phase $CO_2\cdot C_2H_2$ (1:1) that is metastable with respect to bulk CO_2 and bulk C_2H_2 under cryogenic conditions [1,2]. On the KCl(100) surface, CO_2 and C_2H_2 are known to form well-ordered 2D layers with $(6\sqrt{2}\times\sqrt{2})R45^\circ$ and $(\sqrt{2}\times\sqrt{2})R45^\circ$ symmetry, respectively. In coadsorption experiments a KCl(100) surface was precovered with CO_2 at 80 K and then exposed to acetylene and CO_2 at partial pressures of 10^{-8} mbar. LEED patterns and infrared spectra indicate the displacement of the high-order CO_2 layer and the formation of acetylene islands under these conditions. However, previously unobserved IR bands at 2368.6 cm^{-1} (CO_2) and 3192.3 cm^{-1} (C_2H_2) both with dipole moments perpendicular to the surface are a strong indication for the formation of a mixed phase. Results of plane wave DFT calculations are presented which show that the total energy of a $CO_2\cdot C_2H_2$ (1×1)/KCl(100) structure with perpendicularly oriented acetylene on top of Cl^- and CO_2 on top of K^+ is only 1.8 kJ mol^{-1} higher compared to total energies of the separated phases. In addition, phonon calculations based on this structure model can reproduce the observed blue shift (CO_2) and red shift (C_2H_2). [1] T. E. Gough, T. E. Rowat, J. Chem. Phys. **109** (1998), 6809 [2] T. C. Preston, R. Signorell, J. Chem. Phys. **136** (2012), 94510

O 27: Overview Talk: Leonhard Grill

Time: Tuesday 9:30–10:15 Location: S054

Invited Talk O 27.1 Tue 9:30 S054

The Emergence of Covalent On-Surface Polymerization — •Leonhard Grill — Department of Physical Chemistry, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria

The covalent linking of molecular building blocks directly in the two-dimensional confinement of a surface, the so-called on-surface polymerization, has developed rapidly in the last years since it represents a reliable strategy to grow functional molecular nanostructures in a controlled fashion. In this presentation an overview over the growth of such structures will be given, highlighting the important aspects for their formation. These processes are typically studied by scanning tunneling microscopy that allows exploration of the initial monomer species, intermediate products and final nanostructures with sub-molecular spatial resolution. In this way, the chemical structures of the ex-situ synthesized initial molecules are directly correlated with the outcome of the chemical reaction. Examples with different monomer species in view of growing heterogeneous molecular structures and the importance of the molecular interaction with the template surface as a further key parameter to control the molecular diffusion and tune the final molecular architecture will be discussed as well as the functionality of the resulting structures.

O 28: Organic-Inorganic Systems I: PTCDA

Time: Tuesday 10:30–13:00 Location: S054

Invited Talk O 28.1 Tue 10:30 S054

Unravelling the structural and electronic properties of organic/metal interfaces with photoemission tomography — •Peter Puschnig — Institut für Physik, NAWI Graz, Karl-Franzens-Universität Graz, Graz, Austria

In the last years, a renaissance of angle-resolved photoemission spectroscopy (ARPES) for organic/metal interfaces could be observed. This development was mainly driven by the fact that, in opposition to conventional wisdom, the angular dependence of the photoemission current from oriented molecular films can be understood by assuming a plane wave as the final state of the photoemission process. This approximation allows for a simple and intuitive interpretation of the transition matrix element in terms of the Fourier transform of the initial state orbital leading to a combined experimental/theoretical technique, called photoemission tomography (PT).

In this contribution, I will focus on recent experimental and theoretical results obtained by PT. First, on the example of a Cs-doped bilayer of sexiphenyl, I demonstrate how PT enables a layer-resolved picture of the electronic structure thereby revealing the charge transfer processes upon doping. Similarly, for the doping of a monolayer of pentacene on Ag(110), PT unambiguously identifies the electronic states at various doping stages and unravels the processes determining the electronic level alignment. Finally, for the example of a PTCDA monolayer on Ag(110), I will show how ARPES data for a set of photon energies in the range between 20 and 55 eV leads to three-dimensional real-space images of molecular orbitals.

O 28.2 Tue 11:00 S054

Vibronic Modes in Molecular Orbital Imaging — •Achim Schöll[1], Martin Graus[1], Manuel Grimm[1], Christian Metzger[1], Matthias Dauth[2], Christian Tusche[3,4], Jürgen Kirschner[4], Stephan Kümmel[2], and Friedrich Reinert[1] — [1]Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg, Experimentelle Physik 7, 97074 Würzburg — [2]Universität Bayreuth, Theoretische Physik IV, 95440 Bayreuth — [3]Forschungszentrum

Jülich, 52425 Jülich — [4]Max Planck Institut für Mikrostrukturphysik, 06120 Halle

Photoelectron momentum microscopy with high energy resolution allows imaging of molecular orbitals with resolution of vibronic modes. We demonstrate that the intensity patterns of photoelectrons derived for the vibronic sidebands of molecular states show characteristic changes due to the distortion of the molecular frame in the vibronically excited state. By a comparison to the simulated patterns derived from calculations, an assignment of the specific vibronic mode that preferentially couples to the electronic excitation is possible, which in the example of the HOMO of coronene is a b2u inplane mode with an energy of 0.2 eV. Orbital imaging by photoelectron momentum mapping with vibronic resolution thus provides unique information for the analysis of the coupling between electronic and vibronic excitation, and allows fascinating insight into the properties of molecular materials.

O 28.3 Tue 11:15 S054

Surface crystallography by LEED-IV of large organic adsorbates on Ag — •Ina Krieger[1,3], Georg Held[2], Christian Kumpf[3], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn, 53115 Bonn, Germany — [2]Department of Chemistry, University of Reading and Diamond Light Source, UK — [3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52428 Jülich, Germany

LEED-IV is a powerful technique for surface crystallography which supplies detailed experimental structure information on the adsorption geometry of large organic molecules on surfaces revealing important insights in inter-atomic interactions and chemical bonding. Using data from different angles of incidence and optimizing the program code we were able to overcome the challenges given by the limitations of the experimental data set and the calculation times required for the complex and large unit cells.

Here we will report on a recent LEED-IV analysis of PTCDA on Ag(100), at present yielding a good Pendry R-factor of about 0.23. The calculation is based on a unit cell containing 156 atoms and experimental curves for five angles of incidence with an energy-to-parameter ratio over 200 eV. We were able to derive structural information about the surface geometry, in particular with regards to vertical distortions of the molecule core and the buckling of the substrate surface, which could so far not be obtained by other structure methods and are in good agreement with results from DFT and NIXSW studies. Supported by the DFG.

O 28.4 Tue 11:30 S054

Structure and thermal stability of organic heterostructures on Ag(111) — •Sebastian Thussing, Laura Fernandez, and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

The growth of highly ordered molecular films exceeding the first few monolayers represents a challenge as these layers are inherently unstable and susceptible to dewetting processes. Understanding the kinetics of associated phase transformations and proper characterization tools are therefore crucial in such studies. We have investigated the thermal stability and intermixing of various heterolayer model systems (stacked CuPc/PTCDA and TiOPc/PTCDA layers grown on Ag(111)) by means of analyzing the characteristic vibrational modes of these molecules using IR spectroscopy. In addition, SPA-LEED provided information regarding the lateral ordering of these layers. We find that the growth of TiOPc layers on Ag(111) leads to the formation of a stable bilayer where the first layer is oriented with "Ti=O up" and the second layer with "Ti=O down". This particular structural arrangement is attributed to a minimization of dipole-dipole interaction within this stacked Ti=O assembly. Considering the stability of this configuration, bilayers of TiOPc (and CuPc for comparison) have been combined with PTCDA contact primer layers. Again the TiOPc-bilayer exhibits exceptional thermal stability with minimal intermixing with underlying PTCDA/Ag(111) up to about 450K. This is in contrast to the growth of a CuPc bilayer on PTCDA/Ag(111) which shows negligible intermixing but CuPc cluster formation already at T = 250K.

O 28.5 Tue 11:45 S054

Perlyene derivatives adsorbed on O-terminated ZnO. An X-ray standing wave study — •Antoni Franco-Cañellas[1], Jens Niederhausen[2], Alexander Hinderhofer[1], Tien-Lin Lee[3], Alexander Gerlach[1], Norbert Koch[2,4], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany — [3]Diamond Light Source, UK — [4]Institut für Physik, Humboldt-Universität zu Berlin, Germany

Adsorption-induced conformational changes of large organic molecules have been extensively studied in the past for metal-organic interfaces employing the X-ray standing wave (XSW) technique [1], which provides an element-specific measurement of the adsorption distance of the molecule. Here, we show that the same method can be applied to inorganic-organic semiconductor interfaces. In particular, perylene, PTCDA and PTCDI adsorbed on O-terminated ZnO were studied with XSW. Our results shed light on how the ZnO affects the adsorption geometry of the molecule and how different functional groups distort and modify the overall adsorption distance, which is crucial to properly understand the substrate-molecule energy-level alignment within the context of hybrid inorganic-organic systems for optoelectronic applications [2,3].

[1] A. Gerlach et al., in The Molecule-Metal Interface (eds N. Koch, N. Ueno and A. T. S. Wee), Wiley-VCH, Weinheim, Germany (2013).

[2] R. Schlesinger et al. Phys. Rev. B 2013, 87, 155311.

[3] M. Gruenewald et al. J. Phys. Chem. C 2015, 119, 4865.

O 28.6 Tue 12:00 S054

Tracing structural and electronic changes in the first metal layer of metal-organic hybrid interfaces — •Johannes Seidel[1], Norman Haag[1], Lisa Grad[1], Gerben van Straaten[3], Markus Franke[3], Christian Tusche[2], Jürgen Kirschner[2], Christian Kumpf[3], Benjamin Stadtmüller[1], Mirko Cinchetti[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany — [3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany

In this work, we show how the geometric and electronic properties of metal surfaces can be altered by the molecule-substrate interaction. As a model system, we chose a Ag(111) surface and embed Pb tracer atoms into the topmost Ag(111)-layer by surface alloying.

We have studied the electronic valence structure of interfaces formed by prototypical organic molecules adsorbed on the Pb/Ag(111) surface alloy by momentum microscopy. While the adsorption of PTCDA significantly alters the alloy band structure, no changes are observed for CuPc. The changes in the valence band of the PTCDA/Pb/Ag(111) interface can be explained by vertical relaxation of the Pb tracer atoms as determined by x-ray standing waves method. Such relaxation occurs only at the interface formed with PTCDA, not with CuPc. We thus propose that the modifications of the Pb/Ag(111) surface alloy can be attributed to the formation of local bonds between PTCDA and the surface alloy which are absent in case of CuPc.

O 28.7 Tue 12:15 S054

Determination of the adsorption geometry of the PTCDA on the Cu(110) surface by NIXSW triangulation — •Simon Weiss[1,2], Ina Krieger[3], Timo Heepenstrick[3], Serguei Soubatch[1,2], and F. Stefan Tautz[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 — [3]Institut für Physikalische und Theoretische Chemie, Universität Bonn, 53115 Bonn, Germany

The normal incidence x-ray standing wave (NIXSW) technique is frequently used to determine the adsorption height of atoms or molecules adsorbed on surfaces. Moreover it is possible to identify the adsorption site as well using several Bragg reflections and the triangulation approach.

We applied this method to a ordered layer of 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) on the Cu(100) surface. This molecular phase contains two differently orientated PTCDA molecules, equivalent from structure point of view, which are found to be located at bridge sites. Compared to PTCDA adsorbed on the low index Ag surfaces, the bending of the PTCDA molecule on Cu(100) is different. The carboxylic oxygens are no longer located below the perylene backbone. Nevertheless the tendency that the oxygen atoms adsorb close to on top positions relative to the surface atoms is conserved.

O 28.8 Tue 12:30 S054

Controlling the electronic properties of heteromolecular monolayers without affecting their structure through exchange of the phthalocyanine central metal atom — •Gerben van Straaten[1], Benjamin Stadtmüller[2], Markus Franke[1], and Christian Kumpf[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich GmbH, Jülich, Germany, and Jülich-Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Kaiserslautern, Germany

Planar aromatic molecules in a mixed monolayer can indirectly influence each other leading to charge transfer from one molecule to the other via the substrate[1]. This effect provides new ways to tailor the properties of metal-organic interfaces but it's application is complicated by the fact that exchanging the molecular species can change the lateral ordering. This can be avoided when phthalocyanine molecules are used since their interaction with neighboring molecules is largely independent of the central metal atom. Taking advantage of this we prepared mixed monolayers of SnPC and PTCDA on Ag(111) and compared them with known CuPC + PTCDA monolayers exhibiting the same lateral structure[1]. We observed a shift of the PTCDA FLUMO and surprising changes in the vertical adsorption structure, proving that this technique allows tuning of the organic-metal interface properties independently of the lateral structure.
[1] Benjamin Stadtmüller et al., Nature Communications 5 (2014)

O 28.9 Tue 12:45 S054

Understanding the planarization of shuttle-cock shaped subphthalocyanine molecule on Cu(111) surface — •Shashank S. Harivyasi[1], Oliver T. Hofmann[1], Nahid Ilyas[2], Oliver L.A. Monti[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, Austria — [2]University of Arizona, Tucson, Department of Chemistry & Biochemistry, 1306 E. University Blvd., Tucson, AZ 85721, USA

The structure of an organic semiconductor plays a determining role in its adsorption on a metal surface. Large planar molecules like planar phthalocyanines, pentacene and PTCDA typically lie completely flat on most metal surfaces. The situation becomes more complex in case of non-planar molecules. They generally show a tendency to planarize upon adsorption but the extent of this planarization varies from negligible to almost complete for various metal-molecule combinations.

Here, we try to understand the reasons for this planarization by studying an extreme example exhibiting almost complete planarization: adsorption of shuttle-cock shaped Chloroboron subphthalocyanine on Cu (111). Using DFT, we study the steps of the adsorption process by gradually increasing the van der Waals interaction between the adsorbate and the substrate and following the evolution of the molecule's electronic and geometrical structure. We identify the bonding of the molecule as a two-stage process involving Fermi-level pinning followed by a rehybridization of the molecule's frontier orbitals. Especially the observed evolution of charge rearrangements help us to explain why we see an almost complete planarization.

O 29: Topology- and Symmetry-Protected Materials

Time: Tuesday 10:30–13:30 Location: S051

Invited Talk O 29.1 Tue 10:30 S051

Toward single atom qubits on a surface: Pump-probe spectroscopy and electrically-driven spin resonance — •William Paul — IBM Research, San Jose CA, USA

We will discuss the characterization of spin dynamics by pump-probe spectroscopy and the use of gigahertz-frequency electric fields to drive spin resonance of a Fe atom on a MgO/Ag(001) surface. Also, the technical challenges in applying a precise voltage to the tip sample junction across a wide radio-frequency bandwidth will be described. The energy relaxation time, T1, of single spins on surfaces can be measured by spin-polarized pump-probe STM (scanning tunneling microscopy) [1]. To date, the relaxation times reported for Fe-Cu dimers on Cu2N insulating films have been of the order ~100 ns [1]. A three-order-of-magnitude enhancement of lifetime, to ~200 us, was recently demonstrated for Co on a single-monolayer of MgO [2]. Here, we report on the tailoring of the T1 lifetime of single Fe atoms on single- and multi- layer MgO films grown on Ag(001). Next, we demonstrate electron spin resonance of an individual single Fe atom, driven by a gigahertz-frequency electric field applied across the tip-sample junction, and detected by a spin-polarized tunneling current. The principle parameters of the spin resonance experiment, namely the phase coherence time T2 and the Rabi rate, are characterized for Fe atoms adsorbed to the monolayer MgO film.

[1] Loth et al., Science 329, 1628 (2010) [2] Rau and Baumann et al., Science 344, 988 (2014) [3] Baumann and Paul et al., Science 350, 417 (2015)

O 29.2 Tue 11:00 S051

Mesoscopic spin coherence through electron focusing in topological insulators — •Philipp Rüssmann, Phivos Mavropoulos, Nguyen H. Long, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Long coherence lengths of quasiparticles are an essential ingredient for spintronics applications. Motivated by previous experiments [P. Sessi et al, Nat. Comm. 5, 5349 (2014)] we undertook a combined theoretical and experimental study, using density functional theory and STM, where we found standing wave patterns of mesoscopic dimensions around magnetic defects on the surface of Bi$_2$Te$_3$. We identified two necessary conditions for the effect: (i) focusing by the Bi$_2$Te$_3$ Fermi surface due to its hexagonal warping and (ii) large scattering strength of the magnetic defects. We modeled different magnetic defects and analyzed the energy dependence of the scattering properties in the energy range where the shape of the constant energy contour changes from circular over hexagonal to snowflake-like. For the calculation of the electronic structure and scattering properties we employed the full-potential relativistic Korringa-Kohn-Rostoker Green-function method [D.S.G. Bauer, Schriften des Forschungszentrums Jülich, Key Tech. 79 (2014); N. H. Long et al., Phys. Rev. B 90, 064406 (2014)].

We enjoy close collaborations with P. Sessi and M. Bode (Würzburg University) and thank for financial support from the DFG (SPP-1666), the VITI project of the Helmholtz Association and computational support from the JARA-HPC Centre (RWTH Aachen University).

O 29.3 Tue 11:15 S051

Generation of transient photocurrents in the topological surface state of Sb$_2$Te$_3$ bydirect optical excitation with mid-infrared pulses — •Johannes Reimann, Kenta Kuroda, Jens Güdde, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

We combine tunable mid-infrared (MIR) pump pulses with time- and angle-resolved two-photon photoemission (2PPE) to study the ultrafast electron dynamics of the topological surface state (TSS) of Sb$_2$Te$_3$. It is revealed that MIR pulses permit a direct excitation of the unoccupied TSS owing to an optical coupling across the Dirac point. This is in contrast to the delayed filling observed in previous 2PPE experiments on topological insulators with pump photon energies in the visible range. The novel optical coupling provokes asymmetric transient populations of the TSS at $\pm k_{||}$, which mirrors a macroscopic photoexcited electric surface current. By observing the decay of the asymmetric population, we directly investigate the dynamics of the photocurrent in the time domain. We find a long equilibration time of $\tau_k^e = 2.5$ ps for the population at $\pm k_{||}$ that shows no significant change for different sample temperatures of 80 K and 300 K. Considering a Debye temperature of $\theta_\mathrm{D} = 162$ K this result indicates that phonons play only a minor role for the momentum scattering. We suggest that scattering at surface defects is instead the limiting factor for the current lifetime.

O 29.4 Tue 11:30 S051

Time- and angle-resolved two-photon photoemission from p-doped septuple-layered topological insulators — •Sebastian Otto, Jonas Rietsch, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Time- and angle-resolved two-photon photoemission is used to study the electronic structure of septuple-layered antimony telluride crystals of different p-dopings. All surfaces show a topological surface state. The Dirac point is found between $E_\mathrm{F} + 0.38$ eV for GeSb$_2$Te$_4$ and $E_\mathrm{F} + 0.25$ eV for SnBi$_{0.2}$Sb$_{1.8}$Te$_4$. The topological surface state is populated mainly from the conduction band minimum according to the evolution of its temporal population. Similar to the case of $SnSb_2Te_4$ [1], the electrons in the topological surface state decay rather fast into a partially unoccupied valence band maximum depending on the strength of the p-doping.

[1] D. Niesner, S. Otto, V. Hermann and Th. Fauster, Phys. Rev. B **89**, 081404(R) (2014)

O 29.5 Tue 11:45 S051

Controlling the spin-texture of topological insulators with organic molecules — Sebastian Jakobs[1,2], Benjamin Stadtmüller[1], •Dominik Jungkenn[1], Martin Laux[1], Johannes Stöckl[1], Martin Aeschlimann[1], Stefan Mathias[3], and Mirko Cinchetti[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str 46, 67663 Kaiserslautern, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany — [3]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We present a rational design approach to customize the spin texture of surface states of a topological insulator (TI). This approach relies on the extreme multifunctionality of organic molecules that are used to functionalize the surface of the prototypical TI Bi2Se3. For the rational design we use theoretical calculations to guide the choice and chemical synthesis of appropriate molecules that customize the spin texture of Bi2Se3. The theoretical predictions are then verified in angular-resolved photoemission experiments. We show that the surface can be passivated while the Dirac cone can be shifted at will by tuning the strength of the molecule-TI interaction and Rashba-split quantum-well interface states can be created. These tailored interface properties - passivation, spin-texture tuning and creation of hybrid interface states - open a wide field of opportunities for interface assisted molecular spintronics in spin-textured materials.

O 29.6 Tue 12:00 S051

Modulating the spin polarization of photoelectrons from a topological insulator — •Ji Hoon Ryoo and Cheol-Hwan Park — Department of Physics, Seoul National University 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea

It has been predicted that the spin polarization of photoelectrons emitted from a topological insulator is highly tunable so that almost 100 % polarization along any arbitrary direction can be achieved by tuning the polarization of light [1]. There have been a number of experimental confirmations of this photo-induced spin modulation phenomenon [2-6]. Although this photo-induced spin modulation in topological insulators suggests a new kind of spin-polarized electron sources [2], there have been some experimental results that cannot be explained by previous theoretical descriptions [1]. In this presentation, we theoretically investigate photoemission process from topological insulators and interpret the recent experimental observations.

[1] C.-H. Park, S. G. Louie, Phys. Rev. Lett. 109, 097601 (2012).
[2] C. Jozwiak et al., Nat. Phys. 9, 293 (2013).
[3] Z.-H. Zhu et al., Phys. Rev. Lett. 112, 076802 (2014).
[4] Z. Xie et al., Nat. Commun. 5, 3382 (2014).
[5] Y. Cao et al., arXiv:1211.5998v1
[6] J. Sánchez-Barriga et al., Phys. Rev. X 4, 011046 (2014).

O 29.7 Tue 12:15 S051

Dirac Cone Protected by Non-Symmorphic Symmetry and highly dispersive 3D Dirac crossings in ZrSiS — •Leslie Schoop[1], Mazhar Ali[2], Carola Strasser[1], Viola Duppel[1], Stuart Parkin[2], Bettina Lotsch[1], and Christian Ast[1] — [1]Max Planck Insititut für Festkörperforschung, Stuttgart — [2]Max Planck Institut für Mikrostrukturphysik, Halle

Materials harboring exotic quasiparticles, such as Dirac and Weyl fermions have garnered much attention from the physics and material science communities. Here, we show with angle resolved photoemission studies supported by ab initio calculations that the highly stable, non-toxic and earth-abundant material, ZrSiS, has an electronic band structure that hosts several Dirac cones which form a Fermi surface with a diamond-shaped line of Dirac nodes. We also experimentally show, for the first time, that the square Si lattice in ZrSiS is an excellent template for realizing the new types of 2D Dirac cones protected by non-symmophic symmetry and image an unforseen surface state that arises close to the 2D Dirac cone. Finally, we find that the energy range of the linearly dispersed bands is as high as 2 eV above and below the Fermi level; much larger than of any known Dirac material so far. We will discuss why these characteristics make ZrSiS very promising for future applications.

O 29.8 Tue 12:30 S051

2D Dirac cones protected by non-symmorphic symmetry in ZrSiS and ZrSiTe — •Andreas Topp[1], Leslie M. Schoop[1], Carola Strasser[1], Bettina V. Lotsch[1,2,3], and Christian R. Ast[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Department of Chemistry, Ludwig-Maximilians-Universität, D-81377 München — [3]Nanosystems Initiative Munich (NIM) & Center for Nanoscience, D-81377 München

Three-dimensional Dirac semimetals which accommodate massless Dirac and Weyl fermions, have recently become of considerable interest because of their exotic physical properties, e.g. an extremly high mobility and magnetoresistance. A new compound, ZrSiS, hosting a square lattice of Si atoms, has been shown to host 3D Dirac cones at the Fermi level with a very large energy range of linear dispersion [1]. Additionally, a new type of Dirac cone protected by non-symmorphic symmetry has been found to exist below the Fermi level which was predicted theoretically to exist in a square lattice [2]. Here, we show by *ab initio* calculations, that in the compound ZrSiTe this cone is moved to the Fermi level. We present the crystal growth results and show preliminary ARPES data concerning the electronic structure of these two compounds.

[1] L. M. Schoop *et al.*, arXiv preprint arXiv:1509.00861 (2015).
[2] S. M. Young, and C. L. Kane, Phys. Rev. Lett. 115, 126803 (2015).

O 29.9 Tue 12:45 S051

Resonant photoemission of the spin-polarized electronic structure in strongly spin-orbit coupled systems — •Henriette Maass, Hendrik Bentmann, Christoph Seibel, Thiago R. F. Peixoto, and Friedrich Reinert — Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg

Strong spin-orbit coupling leads to a lifting of the spin degeneracy in the electronic structure and the emergence of novel topological phases in non-centrosymmetric environments, such as interfaces or surfaces. Using resonant angle-resolved photoemission experiments (ARPES) we have investigated the spin-polarized electronic structure in the surface alloy $BiAg_2/Ag(111)$ and the topological insulator Bi_2Te_3.

Our data reveals pronounced momentum dependent modulations of the photoemission intensity in the 6p derived surface states of $BiAg_2/Ag(111)$, when the photon energy is tuned across the Bi 5d core level excitation. In particular a complete suppression of spectral weight of spin-up and spin-down valence bands occurs for energies shortly below the Bi $5d_{5/2}$ and the $5d_{3/2}$ core levels, respectively. At the same time a considerable modification of the photoelectron spin-polarization can be observed. We compare these results to the case of the topological insulator Bi_2Te_3, where similar variations in the photoemission intensity occur.

[1] H. Bentmann *et al.*, arXiv 1507.04664

O 29.10 Tue 13:00 S051

Electronic structure and topology of the natural superlattice phase Bi_1Te_1 = $(Bi_2)_1(Bi_2Te_3)_2$ — •Markus Eschbach[1], Martin Lanius[1], Ewa Mlynczak[1], Jens Kellner[2], Chengwang Niu[1], Peter Schüffelgen[1], Mathias Gehlmann[1], Pika Gospodaric[1], Sven Döring[1], Martina Luysberg[1], Gregor Mussler[1], Gustav Bihlmayer[1], Markus Morgenstern[2], Detlev Grützmacher[1], Lukasz Plucinski[1], and Claus M. Schneider[1] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institut, 52425 Jülich, Germany — [2]II. Physikalisches Institut B, RWTH Aachen University, 52074 Aachen, Germany

We report on experimental and theoretical investigations of thin films of Bi_1Te_1 grown on Si(111), being part of the natural supperlattice phase series $[Bi_2]_x[Bi_2Te_3]_y$ with $x = 1$ and $y = 2$. Contrary to the closely related, prototypical 3D strong topological insulator Bi_2Te_3, its electronic strutcture as well as topological properties have not been adressed so far. In this study, we present detailed characterization of the bulk crystal structure by X-ray diffraction and transmission electron microscopy and the surface chemistry by X-ray photoelectron spectroscopy. The rich surface electronic structure, investigated by spin- and angle-resolved photoemission spectroscopy, reveals surface states that can be easily confused with Dirac cone-like topological surface states. However, we will show by experiment and comprehensive ab inito density functional theory calculations that Bi_1Te_1 is a weak topological insulator.

O 29.11 Tue 13:15 S051

Probing the electronic structure of the magnetic topological insulator (BiSbV)$_2$Te$_3$ with soft X-ray photoelectron spectroscopy — •Thiago Ribeiro Fonseca Peixoto[1,3], Mohammed Al-Baidhani[1,3], Henriette Maass[1,3], Christoph Seibel[1,3], Hendrik Bentmann[1,3], Steffen Schreyeck[2,3], Martin Winnerlein[2,3], Stefan Grauer[2,3], Charles Gould[2,3], Karl Brunner[2,3], Laurens Molenkamp[2,3], and Friedrich Reinert[1,3] — [1]EP VII, Fakultät f. Physik u. Astronomie, Uni-Würzburg — [2]EP III, Fakultät f. Physik u. Astronomie, Uni-Würzburg — [3]Röntgen Center for Complex Materials (RCCM), Uni-Würzburg

By means of X-ray photoemission (XPS) and absorption (XAS) spectroscopy we investigated the electronic structure of (BiSbV)$_2$Te$_3$ thin films, a three-dimensional magnetic topological insulator, recently reported as an anomalous quantum Hall system [1]. The films were epitaxially grown on a Si(111) crystal and covered by a Se cap to avoid contamination during exposition to air. After thermally desorbing the Se cap, the core-level lines of the constituent elements and the V $L_{2,3}$ absorption edges were measured for different V concentrations (0, 2 and 4 at.%). Our data evidence the incorporation of Se atoms in the film. By means of resonant photoemission we identify the signature of the V 3d states at the Fermi level, which may contribute to the exotic transport properties of the system. We discuss the chemical environment of the V atoms and show that our techniques are well suited for the study of the electronic properties of this novel class of materials.
[1] C.-Z. Chang *et al.*, Nat. Mat. Lett. **14**, 473 (2015).

O 30: 1D Metal Wires on Semiconductors I

Time: Tuesday 10:30–13:15 Location: S052

O 30.1 Tue 10:30 S052

One dimensional plasmons in Si(hhk)-Au — •Timo Lichtenstein[1], Marvin Detert[1], Julian Aulbach[2], Jörg Schäfer[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Physikalisches Institut and RCCM, Universität Würzburg

For future plasmonic devices the understanding of low dimensional collective excitations is indispensable. For quasi one dimensional (1d) structures Au induced wires on regularly stepped Si(hhk) offer the perfect playground. Therefore, Si(553) and Si(775) were prepared at coverages where both surfaces host a double atomic gold chain per terrace. The wire quality was checked with spot profile analysis in low energy electron diffraction (SPA-LEED). A combination of an electron energy loss spectrometer and SPA-LEED providing both high energy and momentum resolution gave access to the plasmon dispersion.

Although 1d metallicity is observed, the plasmon dispersion strongly depends on a two-dimensional crossover: on the lateral distribution of the 1d electron density of states (DOS) within one terrace (intrawire correlation), as well as on the spacing of the wires (interwire correlation). This can quantitatively be described by a modified plasmon model for a wire array. We obtained effective widths of 7.5 Å for Si(553)-Au and 10.2 Å for Si(775)-Au, which are considerably smaller than the terrace widths. A modulated DOS of comparable width can also be seen by tunneling spectroscopy. These effective widths seem to be influenced both by the structural motif, i.e. single or double chain, as well as by the terrace size.

O 30.2 Tue 10:45 S052

Impurity-mediated early charge density wave condensation in the oxygen-adsorbed In/Si(111)-(4x1)/(8x2) nanowire array — •Stefan Wippermann[1], Andreas Lücke[2], Wolf Gero Schmidt[2], Deok Mahn Oh[3], and Han Woong Yeom[3] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Universität Paderborn, Germany — [3]Pohang University, South Korea

The self-assembled In/Si(111)-(4x1) nanowire array is an extremely popular model system for one-dimensional electronic systems and features a reversible temperature-induced phase transition into a charge density wave (CDW) ordered ground state. While impurities have been widely known to affect this phase transition, the atomistic mechanisms have rarely been elucidated. Here we present a joint experimental and first principles study, demonstrating oxygen impurity atoms to condense the In/Si(111) nanowire array locally into its CDW ground state, even above the transition temperature. Interestingly, CDW ordering is induced only by a concerted effect of multiple impurities. The mechanism is explained as a subtle interplay between coherent superposition of local impurity-induced lattice strain, a strong coupling between electronic and lattice degrees of freedom, and phononic effects on the free energy. Funding from DFG FOR1700 is gratefully acknowledged.

Invited Talk O 30.3 Tue 11:00 S052

Taking Nanoscience to the Edge – The Different Appearances of One-Dimensional Physics — •Jörg Schäfer — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

The technologies to fabricate nanostructures on surfaces with atomic precision have become very elaborate, making it possible to play with low-dimensional physical phenomena: among these, approaches to the one-dimensional (1D) world offer a particularly rich arena. What can we expect here? With the lack of effective screening, and in the presence of quasi-1D electron states that promote particular scattering vectors, these systems become susceptible to symmetry-breaking ground states. Idealized examples include, e.g., Peierls instabilities or magnetic ordering – while in real-word systems these phenomena may be far more complex.

The study of such quasi-1D systems on semiconductor surfaces, i.e., atomic wires, has made tremendous progress in the last years. In my talk I will review some of the most interesting realizations. Specifically, I will address the scenarios encountered for multi-band metallic chains with strong spin-orbit coupling, and their tunability. Moreover, as a recent development, we will turn to the step edges of terraced substrates with honeycomb chains, that show strong indications for spin polarization and long-range magnetic ordering. Such setup has intriguing connections to honeycomb topological insulators, predicted to have 1D edge states. The talk will look at this developing field from an overview perspective.

O 30.4 Tue 11:30 S052

Surface vibrational Raman modes of In/Si(111)-(4x1) and (8x2) nanowires — •Stefan Wippermann[1], Wolf Gero Schmidt[2], Eugen Speiser[3], and Norbert Esser[3] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Universität Paderborn, Germany — [3]ISAS Berlin, Germany

The ordered array of atomic-scale In nanowires that self-assembles on the Si(111) surface is a prototypical model system for one-dimensional (1D) electronic systems. It exhibits a Peierls-like instability, inducing a reversible phase transition from the metallic (4x1) phase into the insulating (8x2) ground state at $T_C = 120$ K. The detailed nature and mechanism of this metal-insulator (MI) transition is still discussed controversially. We performed a joint *first principles* and surface vibrational Raman spectroscopy study of the In/Si(111)-(4x1)/(8x2) surfaces' vibrational properties. The measured phonons are assigned to characteristic modes of the quasi-1D In nanowires, employing density functional theory calculations and symmetry considerations. Both the (4x1) and (8x2) phases exhibit a distinct set of phonon modes. The observed strong modifications in the Raman spectra of the (8x2) phase are consistent with a symmetric quadrupling of the surface elementary cell and confirm characteristic structural changes at the surface. Funding from DFG FOR1700 is gratefully acknowledged.

O 30.5 Tue 11:45 S052

Spin correlations in the Si(553)-Au nanowire system — •B. Hafke[1], T. Frigge[1], B. Krenzer[1], J. Aulbach[2], R. Claessen[2], J. Schaeffer[2], and M. Horn-von Hoegen[1] — [1]Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [2]Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), 97074 Würzburg

To study the microscopic mechanism of formation, stabilization, and interaction in low dimensional systems we used Si(553) as vicinal surface to enforce the nucleation of Au into one dimensional wires. Deposition of 0.5 ML Au results in the formation of one pair of 1D Au atomic chains per Si terrace exhibiting a twofold periodicity. These metallic wires are structurally terminated by Si step edge atoms, which show a threefold periodicity of the Si atoms along the rows. Theory predicts an antiferromagnetic spin ordering of every third Si step edge atom [1]. The long-range interaction of the twofold and threefold periodicity is investigated by spot-profile analysis in SPA-LEED at a sample temperature of 80 K. The strict twofold periodicity of the Au atoms is not correlated between adjacent wires. In contrast the threefold ordering of the Si spins exhibit a clear short range order perpendicular to the Au wires. Both results support the structure model where the interrow correlation is mediated by the spin-spin interaction of adjacent Si step edge atoms.

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. 1, 58 (2010).

O 30.6 Tue 12:00 S052

Interwire coupling of In(4×1) reconstruction probed by transport measurements — •Ilio Miccoli[1], Frederik Edler[1], Stephanie Demuth[1], Herbert Pfnür[1], Stephan Wippermann[2], Andreas Lücke[3], Wolf G. Schmidt[3], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Grenzflächenchemie und Oberflächenphysik, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [3]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

The In(4×1)/Si(111) reconstruction is used as a prototype for the understanding of 1D systems of atomic chains. It shows strong anisotropic transport properties and a temperature driven metal-insulator transition. Although being intensively studied for more than one decade the effect of defects induced by adsorption (e.g. O_2, H_2) are still under current debate. A better understanding of the influence of defects and a correlation with transport measurements can be achieved by a spatial constriction of the electron path. This restriction was realized by optical ex-situ lithography with reactive ion etching. We report a systematic investigation of the confinement effects using a 4-tip STM/SEM system. Moreover, O_2 adsorption dependent transport studies show not only a reduction of conductivity along the direction of atomic chains but also a decrease in the perpendicular. This was not reported before and reveals an effective interwire coupling between the chains, which is in agreement with recent DFT calculations.

O 30.7 Tue 12:15 S052

Phase transition of In-Si(111) (4x1)- (8x2) nanowires in a new light — •Eugen Speiser[1], Stefan Wippermann[2], Simone Sanna[3], Wolf Gero Schmidt[3], Sandhya Chandola[1], and Norbert Esser[1] — [1]ISAS e.V., Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [3]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany

Although recognized as a model case for atomic metallic nanowires, the (4x1)-(8x2) phase transition continues to hide behind the complexity of the structure and electronical properties. In cooperation with continuously developing theoretical methods a variety of conventional and newly developed experimental surface investigation methods are actively applied to elucidate the underlying mechanism of the phase transition. Our approach to this problem is the joint work of calculations and measurements of the low energy surface vibrations localized in the top layer. Successful assignment of calculated vibrational patterns and frequencies to measurements of both the insulating (8x2) and metallic (4x1) phases, is a necessary requirement to understand the dynamics of each phase. Based on this knowledge an interpretation of temperature dependency of phonon frequencies near the phase transition will be given in terms of participation of the electron phonon coupling to the phase transition mechanism. Coupling parameters between phonons and electrons can be estimated from an empirical model based on Landau-Ginsberg theory, as already verified in 1D like bulk materials, eg. blue bronze.

O 30.8 Tue 12:30 S052

Dynamic Ginzburg-Landau theory for the Peierls transition in In/Si(111) — •Yasemin Ergün and Eric Jeckelmann — Leibniz Universität Hannover, Germany

We investigate thermal fluctuations and collective excitations in quasi-one-dimensional charge-density-wave systems using the Ginzburg-Landau (GL) theory. Starting from a microscopic Su-Schrieffer-Heeger-like model for In/Si(111), we generalized the GL theory for grand canonical Peierls transitions. The equilibrium properties and the non-equilibrium dynamics are simulated using the Langevin approach. We discuss our theoretical results in relation to doping and spectroscopy experiments for In/Si(111). Support from the DFG through the Research Unit FOR 1700 is gratefully acknowledged.

O 30.9 Tue 12:45 S052

Beyond thermal equilibrium: ultrafast non-thermal melting of a surface CDW in the In/Si(111) atomic-wire system — •Tim Frigge, Bernd Hafke, Tobias Witte, Boris Krenzer, and Michael Horn-von Hoegen — Department of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

The wire-type arrangement of Indium atoms on a Silicon(111) surface serves as a famous prototype for the formation of a quasi one-dimensional charge density wave groundstate. We used time-resolved electron diffraction in surface-sensitive geometry to investigate the transient non-equilibrium dynamics of the impulsively driven (8x2)→(4x1) phase transition. Optical excitation of the (8x2) groundstate with fs-laser pulses revealed the existence of a metastable, supercooled (4x1) excited state at 30 K. This phase survives for hundreds of picoseconds because the recovery of the (8x2) phase is hindered due to an energy barrier of 40 meV. At fluences of 3-7 mJ/cm^2 the CDW groundstate is lifted and the structure changes within 350 fs. This photoinduced transition can not be explained by a simple thermal excitation scenario because laser induced heating takes place on timescales 6 times longer. Instead, we explain the observed dynamics through an accelerated displacive excitation scenario upon changes of the potential energy landscape. This also explains the observation of an increase of the excitation time constant towards lower fluences below 3 mJ/cm^2.

O 30.10 Tue 13:00 S052

Atomistic Mechanism and Dynamics of the Optically Induced In/Si (111) (8x2)-(4x1) Phase Transition — •Andreas Lücke[1], Simone Sanna[1], Uwe Gerstmann[1], Stefan Wippermann[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Interface Chemistry and Surface Engineering Department Max-Planck-Institute for Iron Research GmbH, 40237 Düsseldorf, Germany

The In-Si(111)(8x2)/(4x1) nanowire array features a Peierls instability-driven phase transition, the mechanism of which has been controversial since its discovery, cf. Ref. [1-3]. Experimentally it has been shown that the insulating (8x2) phase undergoes a phase transition towards the metallic (4x1) phase upon optical excitation far below the critical temperature [4]. Here we rationalize this finding by means of ab-initio total-energy and electronic-structure calculations and provide atomistic insight into the driving force and the dynamics of the optically driven phase transition by performing molecular dynamics simulations on excited-state potential energy surfaces. In particular we relate the phase transition to the population/depopulation of specific surface bonds that excite soft phonon modes. Our results rationalize recent findings from ultra-fast time-resolved electron diffraction.

1. H. W. Yeom, et al. Phys. Rev. Lett. 82, 4898 (1999).
2. J. R. Ahn, et al. Phys. Rev. Lett. 93, 106401 (2004).
3. S. Wippermann, et al., Phys. Rev. Lett. 105, 126102 (2010).
4. S. Wall et al., Phys. Rev. Lett. 109, 186101 (2012).

O 31: Heterogeneous Catalysis: Theory

Time: Tuesday 10:30–13:00 Location: S053

O 31.1 Tue 10:30 S053

Analyzing the case for bifunctional catalysis — •Mie Andersen[1], Andrew J. Medford[2,3], Jens K. Nørskov[2,3], and Karsten Reuter[1] — [1]Theoretical Chemistry, Technische Universität München, Germany — [2]SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, CA, USA — [3]Department of Chemical Engineering, Stanford University, CA, USA

Computational screening based on scaling relations has proven highly successful in rationalizing, why efficient catalysts are often found within only a narrow range of binding energies that allow the dissociation of reactants without hindering the formation of products [1]. It has been suggested that these severe limitations in material space could be overcome by bifunctional catalysts, which couple two active sites, each catalyzing a particular reaction step. Using global optimization techniques and microkinetic modeling in the mean-field (MF) approximation, we explore the theoretical limits for such a bifunctional gain for a wide range of model reactions. This analysis suggests that bifunctional catalysts made from two active sites of similar type, i.e. controlled by similar scaling relations, will in general not reach higher activities than single-site catalysts. We correspondingly aim to quantify how "different" the two active sites must be in order for the idea of bifunctionality to work.

[1] J. K. Nørskov et al., Nature Chem. 1, 37 (2009)

O 31.2 Tue 10:45 S053

NO-induced inhibition of oxide formation on Pd catalysts: A first-principles kinetic Monte Carlo study — •Juan Manuel Lorenzi[1], Sebastian Matera[2], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Freie Universität Berlin, Germany

In the context of NO_x Storage Reduction (NSR) catalysts, in which oxidation of NO into NO_2 is a critical intermediate step, interest shifts to understanding the oxidation properties of typically employed Pt-group catalysts under the simultaneous exposure to CO, NO and O_2. We assess this for a model Pd(100) catalyst by means of a comprehensive first-principles kinetic Monte Carlo study, which is based on an extensive set of density-functional theory derived rate constants and which explicitly resolves lateral interactions among all surface species. Multiple studies on Pd(100) in a pure CO + O_2 atmosphere had indicated a strong propensity to surface oxide formation under technologically relevant gas-phase conditions (e.g. [1]). In contrast to this we find that already small amounts of NO in the feed lead to a substantial reduction of the O coverage even in oxygen-rich environments. While NO thus efficiently inhibits oxide formation, the total activity of the resulting metal surface towards NO (and CO) oxidation is still comparable to the one predicted previously for the oxidized surface [2]. [1] S. Blomberg *et al.*, Phys. Rev. Lett. **110**, 117601, (2013). [2] J. Jelic, K. Reuter, and R. Meyer, Chem. Cat. Chem. **2**, 658 (2010).

O 31.3 Tue 11:00 S053

First-principles computational screening of dopants to improve the Deacon process over RuO_2(110) — •Zhen Yao, Farnaz Sotoodeh, and Karsten Reuter — TU München, Germany

Cl_2 is widely used in many chemical industries which produce HCl as byproduct. Recycling HCl back to high purity Cl_2 is therefore mandatory for a sustainable operation. RuO_2 shows unique activity for the corresponding route along the Deacon process, i.e. the catalytic oxidation of HCl to chlorine and water.

One possibility to further improve this performance is a doping of the oxide matrix. With the aim of guiding experimental activities through chemical compound space, we perform a density-functional theory based computational screening study over a wide range of transition metal dopants. Previous work suggested the chlorine desorption from the surface as a rate-controlling step [1,2]. We correspondingly employ the Cl adsorption energy and dopant segregation energy as descriptors to assess activity and stability. Among the metals screened, Cu, Ag, and Zn emerge as most promising dopants.

[1] S. Zweidinger *et al.*, J. Phys. Chem. C. **112**, 9966 (2008).
[2] A. P. Seitsonen *et al.*, J. Phys. Chem. C. **114**, 22624 (2010).

O 31.4 Tue 11:15 S053

Embedding of Vanadium Atoms into the Anatase TiO2(101) Surface — Stig Koust[1], Logi Arnarson[1,2], Paul Georg Moses[2], Igor Beinik[1], Zheshen Li[1], Jeppe Vang Lauritsen[1], and •Stefan Wendt[1] — [1]Interdisciplinary Nanoscience Center (iNANO) and Department of Physics and Astronomy, Aarhus University, DK-8000 Aarhus C, Denmark — [2]Haldor Topsøe Research Labs, DK-2800 Lyngby, Denmark

Selective catalytic reduction (SCR) catalysis is widely used to reduce NOx into N2 and H2O in flue and exhaust gasses, often using ammonia (NH3) as H source. SCR reactions are best catalyzed by anatase TiO2-supported submonolayer VOx-catalysts that are promoted with W and/or Mo. Here we present atomically resolved STM images of sub-monolayer V on anatase TiO2(101). Following V deposition at 100 K, the surface was covered with small isolated V clusters that were distributed homogeneously on the terraces. Our STM studies revealed an embedding of V into the near-surface region upon warming the sample to room temperature. A significant decrease in the density of V clusters was observed and new features in the STM images appeared, which we assign to monomeric V at regular Ti surface sites. Thus, surface Ti atoms are substituted by V atoms. Additional XPS characterization revealed the oxidation state of V being 2+ directly after deposition at 100 K, indicating a preferred binding between V clusters and surface O atoms. Characteristic changes were observed in the V 2p region after warming the sample to room temperature, corroborating our STM data.

O 31.5 Tue 11:30 S053

Hydrogen coadsorption effects on C-C bond formation on Ru(0001) at realistic temperatures and pressures: An ab initio study — •Xunhua Zhao, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

Hydrogen coadsorption is a crucial component of heterogeneous catalysis of hydrocarbons. Our recent study [1] demonstrated the critical role of hydrogen coadsorption in the stabilization of CH_2 species on the Ru(0001) surface. In the present work, we report a DFT-PBE study of hydrogen coadsorption effects on C-C bond formation reactions at realistic conditions up to typical temperature and hydrogen pressure of Fischer-Tropsch synthesis (FTS) [2]. *Ab initio* atomistic thermodynamics is employed to assess the relative thermo-stability of CH_x species, and the string method is used to evaluate the minimum-energy paths for C-C bond formation. CH_x+CH_y and CH_x+C_2H_z ($x, y = 1, 2, 3$ and $z = 3 - 6$) coupling reactions at the monolayer coverage for coadsorbed hydrogen plus reactants are studied to identify possible chain-growth paths in FTS. For comparison, coupling reactions without hydrogen coadsorption are also calculated. It is found that in general hydrogen coadsorption shifts the relative stability to more hydrogen-saturated species (larger x in CH_x for instance). Hydrogen coadsorption is found to have a profound influence on the C-C coupling reaction barriers: While it generally reduces all the barriers, some reaction paths become more favoured in the presence of the coadsorbed hydrogen. — [1] H. Kirsch, X. Zhao et. al., *J. Catal.* **320**, 89 (2014); [2] R. A. Van Santen et. al., *Adv. Catal.* **54**, 127 (2011)

O 31.6 Tue 11:45 S053

CH_2 stabilization and dissociation at steps on Ru(0001) in UHV — •Harald Kirsch, Xunhua Zhao, Sergey Levchenko, and R. Kramer Campen — Fritz-Haber-Institut Berlin, Faradayweg 4-6, 14195 Berlin

In this study we investigated the dissociation of defect(step) bonded CH_2, produced by methane dissociation on Ru(0001) under UHV conditions. Dissociated sticking of CH_4 was performed by using a supersonic molecular beam source. By using vibrational sum frequency generation(SFG) spectroscopy, we found the characteristic CH-stretch vibration of step adsorbed CH_2 at $2925 cm^{-1}$. The observed species saturated at coverages of about 3-5% of a monolayer of carbon. An Arrhenius analysis of the temperature dependent stability gave an activation energy for the depletion of our signal of 45 kJ/mol. This value is 3 times higher than the calculated dissociation barrier of isolated CH_2 at terrace sites. DFT calculations, performed on this system rationalize this observation by a two step process. First by the diffusion and subsequent dissociation of CH_2 to CH + H, when moving from a step to a nearby terrace site(barrier $\approx$ 14 kJ/mol). This CH stabilizes remained CH_2 at steps, produced by ongoing dosing of methane, by increasing the combined diffusion and dissociation barrier to $\approx$ 37 kJ/mol. These results may contribute to a better understanding of the active species in the Fischer-Tropsch Synthesis.

O 31.7 Tue 12:00 S053

Decomposition of formic acid on Pd-Au surfaces — •Holger Euchner, Jan Kucera, and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

Pd-based catalysts have shown promising activity towards heterogeneous [1] and electrochemical [2] dehydrogenation of formic acid (FA), envisioned to be integrated into future H_2 energy technologies. However, the performance of current catalysts so far has not met the technological demands and, unfortunately, rational strategies towards better catalysts are not easy to establish. This is, despite the apparent simplicity of the overall reaction, mainly due to complexity of FA decomposition.

To provide insight into underlying mechanisms and potential for improvement, we have conducted a computational study of the decomposition of FA on Pd-based surfaces. Using dispersion corrected periodic density functional theory (DFT-D3), the effect of replacing sub-surface Pd by Au is investigated. The impact of changing electronic structure on the decomposition pathway of FA, caused by the vertical ligand effect, is studied and discussed with respect to desired dehydration and undesired dehydrogenation reaction. In a further step, to approach a more realistic modeling, the effect of hydrogen as a co-adsorbent, being at the same time a reaction intermediate, is studied.

[1] Grasemann et al., Energy Environ. Sci. **5**, 8171 (2012).
[2] Jiang et al., Phys. Chem. Chem. Phys. **16**, 20360 (2014).

O 31.8 Tue 12:15 S053

Formic acid dehydrogenation over Au/CeO$_2$ catalysts: Theoretical DFT study — •Jan Kučera and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

Heterogeneous catalysts based on nano-sized Au supported on various oxides (e.g., TiO$_2$,CeO$_2$, or SiO$_2$) can selectively decompose formic acid (FA) to provide pure hydrogen already at low temperatures - a process of high technological relevance in the context of hydrogen technology as part of a sustainable energy concept. Despite of the activity ascribed to Au, the decomposition mechanism depends strongly on the nature of the oxide. Unfortunately, the mechanistic understanding of the function of the support remains unclear, which hampers to establish a route towards better catalysts.

Our computational study focuses on the elucidation of elementary processes behind the FA decomposition over Au/CeO$_2$. In particular, the reducible surface of CeO$_2$ facilitates the dynamical formation of catalytically active subnanometer/atomic Au species detached from Au-nanoparticles [1]. We have employed periodic DFT+U models together with a periodic embedded cluster method (PEECM) to investigate the dehydrogenation process of FA over single-Au species on CeO$_2$. We will discuss the influence of the charge transfer between Au and the CeO$_2$ support on the catalytic mechanism in the presence of various surface defects.
[1] N. Yi *et al.*, ChemSusChem **6**, 816 (2013) 816; Y-G. Wang *et al.*, Nat. Commun. **6**, 6511 (2015).

O 31.9 Tue 12:30 S053

(Meta)stability and Dynamics of Nanoclusters at Finite-Temperature — •Diego Guedes-Sobrinho[1], Juarez L. F. Da Silva[1], Ian Hamilton[2], and Luca Ghiringhelli[3] — [1]University of Sao Paulo, Sao Carlos, Brazil — [2]Wilfrid Laurier University, Waterloo, Ontario, Canada — [3]Fritz Haber Institut der MPG, Berlin, Germany

Due to their catalytic properties, transition-metal nanoclusters have been the focus of a large number of experimental and theoretical studies. However, an atomistic understanding of the temperature effects on their structure are far from satisfactory. In this work, we investigate the (meta)stability and dynamics of Au nanoclusters in a range of sizes where a core-shell structure starts to be formed, namely in the range from 25 to 40 atoms. We use ab initio molecular dynamics combined with replica-exchange techniques, in order to obtain an unbiased statistical sampling of the phase space. The energy and forces are described via the PBE exchange-correlation functional, including many-body dispersion interactions [1], as implemented in the all-electron, full potential, numeric atom-centered orbital based FHI-aims package. We find that at room and higher temperature, the gold clusters at the chosen sizes exhibit a dynamical core-shell structure, with a (typically) tetrahedral core loosely bound to the outer liquid-like shell. A suitable structural descriptor, based on the radial distribution function referred to the cluster's center-of-mass, is introduced, in order to capture the invariants along the dynamics of these structures. [1] A. Tkatchenko *et al.*, J. Chem. Phys., **138**, 074106 (2013).

O 31.10 Tue 12:45 S053

Methanol synthesis over Cu/ZnO from molecular dynamics — Luis Martínez-Suárez, Niklas Siemer, •Johannes Frenzel, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany

In the industrial process of methanol synthesis from CO$_2$ the presence of dynamical morphological changes is believed to explain the superior performance of the Cu/ZnO catalyst material under reaction conditions. Yet, a highly corrosive syngas atmosphere at elevated temperatures and pressures substantially hampers *in situ* experimental access to identify the underlying reaction mechanisms and active site(s). Using our combined approach [1,2] of advanced *ab initio* molecular dynamics and thermodynamically optimized catalysts models [3,4] a huge space of possibilities emerging from the structural and chemical configurations of both, adsorbates and continuously altering Cu/ZnO catalyst material, is successfully explored by pure computational means.[5] Extensive sampling of the underlying free energy landscape discloses an overwhelmingly rich network of parallel, competing and reverse reaction channels that interconnect a host of C$_1$ species. Cu/ZnO interface sites and the near surface region over the catalyst surface were identified as key to some pivotal reaction steps in the global reaction network which, ultimately, embodies also important side reactions and catalyst deactivation. Refs.: [1] Frenzel, J. *et al.*, PSS B 250, 1174, [2] Frenzel, J., Marx, D, JCP 141, 124710 [3] Martínez-Suárez, L. *et al.*, PRL 110, 086108 [4] Martínez-Suárez, L. *et al.*, PCCP 16, 26119 [5] Martínez-Suárez, L. *et al.*, ACS Catal. 5, 4201

O 32: 2D Materials I: Structure and Electronic Properties

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

O 32.1 Tue 10:30 H24

Structural and electronic properties of epitaxial multilayer *h*-BN on Ni(111) — Alexander Tonkikh[1], Elena Voloshina[2], Peter Werner[1], Horst Blumtritt[1], Boris Senkovskiy[3], Gernot Güntherodt[1,4], Stuart Parkin[1], and •Yuriy Dedkov[5,6] — [1]MPI Halle (Saale), Germany — [2]HU Belin, Germany — [3]TU Dresden, Germany — [4]RWTH Aachen, Germany — [5]SPECS GmbH, Germany — [6]IHP Frankfurt (Oder), Germany

Hexagonal boron nitride (*h*-BN) is a promising material for implementation in spintronics due to a large band gap, low spin-orbit coupling, and a small lattice mismatch to graphene and to close-packed surfaces of fcc-Ni(111) and hcp-Co(0001). Epitaxial deposition of *h*-BN on ferromagnetic metals is aimed at small interface scattering of charge and spin carriers. We report on the controlled growth of *h*-BN/Ni(111) by means of molecular beam epitaxy (MBE). Structural and electronic properties of this system are investigated using cross-section transmission electron microscopy (TEM) and electron spectroscopies which confirm good agreement with the properties of bulk *h*-BN. The latter are also corroborated by density functional theory (DFT) calculations, revealing that the first *h*-BN layer at the interface to Ni is metallic. Our investigations demonstrate that MBE is a promising, versatile alternative to both the exfoliation approach and chemical vapour deposition of *h*-BN.

O 32.2 Tue 10:45 H24

Structural, thermodynamic and electronic properties of two-dimensional SiC, SiGe, and GeC alloys — Ivan Guilhon[1], Friedhelm Bechstedt[2], •Ronaldo Rodrigues Pela[1,3], Marcelo Marques[1], and Lara Kuhl Teles[1] — [1]Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany — [3]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

We investigate structural, thermodynamic, electronic properties of 2D binary alloys made from graphene, silicene and germanene by means of density functional theory calculations and a statistical method that accounts for disorder and compositional effects. The GGA-1/2 method [1] is used in electronic properties calculations to approximately include quasiparticle corrections. $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ is the only stable alloy at usual growth temperatures. In $\mathrm{Ge}_{1-x}\mathrm{C}_x$, strong distortions of the lattice lead to a pronounced tendency for phase separation. $\mathrm{Si}_{1-x}\mathrm{C}_x$ presents an ordered structure with composition $x = 0.5$ stable up to $T \approx 1000$ K. While $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ and $\mathrm{Ge}_{1-x}\mathrm{C}_x$ are found to have vanishing band gaps, $\mathrm{Si}_{1-x}\mathrm{C}_x$ has, around $x = 0.5$, an appreciable band gap, which decreases exponentially with the growth temperature from ~ 2.2 eV at 300 K to ~ 1.2 eV at 900 K [2].
[1]: Phys. Rev. B 78, 125116 (2008); [2]: Phys. Rev. B 92, 075435 (2015).
Acknowledgments: "Conselho Nacional de Desenvolvimento Científico

e Tecnológico" (CNPq), "Coordenação de Aperfeiçoamento de Pessoal de Nível Superior" (CAPES) and "Alexander von Humboldt Stiftung".

O 32.3 Tue 11:00 H24

Unoccupied states in silicene nanoribbons on Ag(110) — •Nils Fabian Kleimeier, Luca Bignardi, and Helmut Zacharias — Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Unoccupied electronic states of silicene nanoribbons grown on Ag(110) were measured by inverse photoemission (IPE) in ultra-high vacuum conditions. The IPE setup consisted of a modified Erdmann-Zipf electron gun and an acetone filled Geiger-Müller tube with a CaF2 window acting as a bandpass filter. Three individual unoccupied states can be distinguished at 0.3, 0.9 and 1.4 eV above the Fermi level. To investigate occupied states of the nanoribbons, two-photon photoemission at a photon energy of $h\nu = 3.15$ eV was employed. Occupied states associated with the nanoribbons were only visible in spectra excited with p-polarized light. Electron dynamics of the lowest unoccupied state of the nanoribbons at $E - E_F = 0.3$ eV were measured by time-resolved three-photon photoemission at the same photon energy. The lifetime of the state was determined to $\tau = 20$ fs.

O 32.4 Tue 11:15 H24

Absence of Dirac cones in monolayer silicene and multilayer Si films on Ag(111) — •Paolo Moras[1], Sanjoy K. Mahatha[1], Polina M. Sheverdyaeva[1], Valerio Bellini[1,2], Claudia Struzzi[3], Luca Petaccia[3], Tevfik O. Mentes[3], Andrea Locatelli[3], Roberto Flammini[4], Karsten Horn[5], and Carlo Carbone[1] — [1]Istituto di Struttura della Materia - CNR, Trieste, Italy — [2]Istituto di Nanoscienze - CNR, Modena, Italy — [3]Elettra Sincrotrone Trieste, Trieste, Italy — [4]Istituto di Struttura della Materia - CNR, Roma, Italy — [5]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Monolayer silicene and multilayer silicon films on Ag(111) have been subject of many investigations within the last few years. For both systems, photoemission data have been interpreted in terms of linearly dispersing bands giving rise to the characteristic *Dirac cone* feature in the valence band. Here we show, on the basis of angle-resolved photoemission data and ab-initio calculations [1,2] that this assignment is not correct. In monolayer silicene the *Dirac cone* feature is caused by an Ag-derived interface state, while multilayer Si films exhibit a clear diamond-like structure and bulk-like Si bands. These results question the validity of the claim that graphene-like 2-D silicon and silicene multilayers are in fact formed on Ag(111).

[1] P. Moras et al., J. Phys.: Condens. Matter 26, 185001 (2014).

[2] S. K. Mahatha et al., Phys. Rev. B 89, 201416(R) (2014).

O 32.5 Tue 11:30 H24

Low energy electron diffraction and angle resolved photoemission studies of Sn/Au(111) reconstructed surfaces — •Mahalingam Maniraj[1], Sebastian Emmerich[1], Dominik Jungkenn[1], Sebastian Jakobs[1], Benjamin Stadtmüller[1], Mirko Cinchetti[1], Stefan Mathias[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Recent experimental realization of Stanene, a two dimensional allotrope of Sn in a graphene-like structure, has motivated intense research on related Sn based ultrathin materials. We have investigated the growth of Sn on Au(111). Using low energy electron diffraction (LEED) and angle-resolved photoemission spectroscopy, we found five surface reconstructions, each with a distinct band structure. Starting from a coverage of 0.3 monolayers, Sn forms a $(\sqrt{3} \times \sqrt{3})$R30° surface alloy which transforms into a complex superstructure for higher Sn coverages. An angle-resolved photoemission study shows inverted V-shaped bands which are symmetrically centered at the Gamma-point. Additionally, we observed states with parabolic dispersion showing a Rashba-type spin splitting. A direct comparison between our experimental results and band structure calculations will allow us to discuss the formation of Stanene-like band dispersions for these Sn/Au reconstructed surfaces.

O 32.6 Tue 11:45 H24

Molecular interactions to control characteristics of transition metal dichalcogenide based atomically thin field effect devices — •Antony George[1], Sina Najmaei[2], Andreas Winter[1], Zian Tang[1], David Kaiser[1], Uwe Hübner[3], Pulickel Ajayan[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena — [2]Department of Materials Science and Nano Engineering, Rice University, Houston — [3]Leibniz Institute of Photonic Technology, 07702 Jena

Atomically thin field effect transistors (FET) based on monolayer transition metal dichalcogenides have been attracted an immense research interest recently due to their application potential in ultrathin, lightweight transparent device technology. Here we discuss the possibility to tailor the characteristics of monolayer molybdenum disulphide (MoS2) based FET devices using molecular interactions. We have used self-assembled monolayers (SAMs) to control the surface chemistry of the interface between the semiconducting channel and the gate oxide [1]. Therewith such device parameters like mobility, threshold voltage, carrier density can be tuned. We further extend this concept to the development of FETs, which can be tuned by optically switchable molecules. To this end, we fabricated van der Waals heterostructures using MoS2 and carbon nanomembrane (CNM) [2] functionalized with optically switchable molecules. These devices can have different operational modes depending on the type of molecular switching which is triggered by external optical stimulation. [1] Nano Letters 14, 1354 (2014) [2] Prog. Surf. Sci. 87, 108 (2012)

O 32.7 Tue 12:00 H24

Spatial conductivity mapping of unprotected and capped black phosphorus using microwave microscopy — Pieter J. de Visser[1,2], Rebekah Chua[1,3], Joshua O. Island[1], Matvey Finkel[1,4], Allard J. Katan[1], •Holger Thierschmann[1], Herre S.J. van der Zant[1], and Teun M. Klapwijk[1,4] — [1]Kavli Insitute of Nanoscience, Faculty of Applied Sciences, Delft University of Technology, The Netherlands — [2]Department of Quantum Matter Physics, University of Geneva, Switzerland — [3]Department of Physics, National University of Singapore, Singapore — [4]Physics Department, Moscow State Pedagogical University, Russia

Within the family of 2D materials thin flakes of black Phosphorus (bP) play a special role due to their tuneable direct bandgap and high carrier mobilities. Under ambient conditions, however, degradation changes the electronic properties of bP dramatically within hours [1]. Hence, applying protection measures is essential. We compare different protecting layers by measuring the local conductivity of bP flakes over time with scanning microwave impedance microscopy (sMIM). This novel AFM-based technique [2] probes the local sheet resistance with high spatial resolution and even for buried layers. For a bare bP flake we observe drastic changes in conductivity within 24 h. Coverage with 10 nm of HfOx delays degradation. The bP flake is stable for more than a week. Boron Nitride flakes appear to be less effective as a protection. sMIM reveals that here degradation starts at the edges and evolves over days, indicating a diffusive process. [1] Island J O, et al. 2DMat 2, 011002 (2015). [2] K. Lai, et al. Rev Sci Inst 79, 063703 (2008).

O 32.8 Tue 12:15 H24

Coulomb interaction in transition metal dichalcogenides: effects on many-body instabilities — •Gunnar Schönhoff[1,2], Malte Rösner[1,2], Stephan Haas[3], and Tim Oliver Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany — [3]Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484, USA

We develop a material realistic, microscopic model to describe the Coulomb interaction in a TMDC monolayer, focussing on molybdenum disulfide under electron doping. Starting from ab initio Coulomb interaction for the undoped system, we calculate values for the screened matrix elements in real space and see how the interaction becomes more localized with doping. Additionally, we obtain the doping dependend electron-phonon matrix elements and observe a Charge Density Wave instability at high doping.

To quantify the influence of the Coulomb interaction on the superconducting phase, we calculate the Morel-Anderson coefficient μ^*. In contrast to the frequent use of μ^* as a fit parameter or a constant, this leads to a decrease of μ^* with electron doping from 0.25 to 0.1. The influence of the Coulomb interaction turns out to be most important at the boundary between the metallic and the superconducting phase where it delays the phase transition. We argue that the character of the superconducting phase in MoS_2 is phononic.

O 32.9 Tue 12:30 H24

The electronic structure of a 2D MoS_2-WSe_2 heterojunction investigated with photoemission spectroscopy — •Mathias Gehlmann[1], Markus Eschbach[1], Pika Gospodaric[1], Ewa Mlynczak[1], Sven Döring[1], Philipp Nagler[2], Tobias Korn[2], Christian Schüller[2], Slavomír Nemšák[1], Lukasz Plucinski[1], and Claus M. Schneider[1] — [1]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Department of Physics, University of Regensburg, D-93040 Regensburg, Germany

Heterostructures built from van der Waals materials are considered excellent candidates for next generation electronic devices that could overcome the restrictions of classical, Si-based electronics. The weak interlayer interaction in such heterostructures leaves the electronic properties of their building blocks largely intact. Nevertheless, by combining the two different transition metal dichalcogenides (TMDCs) MoS_2 and WSe_2, we produced a two-dimensional p-n junction, with drastically different optical and transport properties compared to the isolated TMDC monolayers and studied the influence of the interlayer coupling on the electronic structure in this novel, two-dimensional heterojunction.

By using photoemission spectroscopy we investigated the band alignment in the two materials. In order to directly observe the electronic band dispersion from micrometer-size flakes we performed k-space microscopy employing a photoemission microscope in angular resolved mode.

O 32.10 Tue 12:45 H24

Superconductivity in the ferecrystals $(PbSe)_{1.14}(NbSe_2)_n$ — •Corinna Grosse[1], Matti B. Alemayehu[2], Matthias Falmbigl[2], Olivio Chiatti[1], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene, OR, 97401, USA

The ferecrystals $(PbSe)_{1.14}(NbSe_2)_n$ are artificially layered materials consisting of n $NbSe_2$ single-layers stacked alternately with atomic double layers of PbSe. $NbSe_2$ is a transition metal dichalcogenide with interesting electrical properties such as superconductivity and charge density waves. The influence of turbostratic disorder, a random rotation between the $NbSe_2$ and PbSe layers, on the superconducting transition temperature has been unknown so far.

We investigate the structural and temperature-dependent electrical properties of the ferecrystals $(PbSe)_{1.14}(NbSe_2)_n$ by means of scanning transmission electron microscopy, X-ray diffraction, in-plane resistivity and Hall measurements and compare them to those of analogous non-disordered misfit layer compound (MLC) polymorphs. We observe a superconducting transition in the resistivity of the ferecrystals. The transition temperatures are reduced by up to 55 % with respect to the analogous MLC polymorphs. This indicates that turbostratic disorder substantially weakens the electron-phonon coupling in $(PbSe)_{1.14}(NbSe_2)_n$. We discuss the results of the structural and electrical properties of the ferecrystals with respect to their MLC analogues and also with respect to ultra-thin $NbSe_2$ layers.

O 33: Photonics and Nanooptics I: Infrared Spectroscopy

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

O 33.1 Tue 10:30 H4

Directional Pt-Re nano-antennas for surface-enhanced Raman spectroscopy of suspended ultraclean carbon nanotubes — •Christian Bäuml, Nicola Paradiso, Tobias Korn, Christian Schüller, and Christoph Strunk — University of Regensburg

We developed a new kind of directional optical nano-antennas based on arrays of nano-strips of platinum-rhenium bilayers. The arrays are designed in order to display a plasmonic resonance when excited with light at around 633 nm with polarization directed orthogonally to the strips. We demonstrate that these structures retain their plasmonic resonance even if subjected to very high temperatures (850°C). This feature allowed us to dramatically amplify the Raman signal on carbon nanotubes (CNTs) grown on top of the antennas via chemical vapor deposition. Such overgrowth technique is nowadays the standard method to produce clean devices for quantum transport experiments. Our antennas are thus a promising building block for hybrid devices that enable amplification of optical signals detected on the very CNT portion investigated in transport experiments by the same device.

O 33.2 Tue 10:45 H4

Plasmonic Enhancement of Infrared Vibrational Signals: Nanoslits versus Nanorods — •Christian Huck[1], Jochen Vogt[1], Michael Sendner[1,2], Daniel Hengstler[1], Frank Neubrech[1,3], and Annemarie Pucci[1,2] — [1]Kirchhoff Institute for Physics, Heidelberg — [2]InnovationLab GmbH, Heidelberg — [3]4th Physics Institute and Research Center SCoPE, Stuttgart

We report on investigations of nanoslit arrays as a substrate for surface-enhanced infrared absorption (SEIRA). Nanoslits, fabricated by electron beam lithography and subsequent argon ion etching, feature strong resonances in the infrared spectral range, according to Babinet's principle. The plasmonic resonances are compared to those of solid nanoantennas, with exactly the same dimensions. Compared to the nanoantenna, a nanoslit can feature several advantages, as will be discussed in the talk. The SEIRA performance is compared by investigating a monolayer of octadecanethiol. Furthermore, the slit geometry is optimized by systematically examining all important parameters. We show, that the slit width has a strong influence on the near-field intensity and therefore also on the SEIRA performance. Finally, the transversal and longitudinal coupling of nanoslits is studied and the response is compared to the excitation of a single nanoslit. A strong coupling behavior is observed, and the periodicity is optimized, leading to the maximum SEIRA signal. The coupling condition is compared to that of solid nanostructures, revealing several differences. Our results give access to general design rules for any sensing application based on the use of inverse nanostructures.

O 33.3 Tue 11:00 H4

Monocrystalline Gold Structures Applied for SEIRA Spectroscopy — •Jochen Vogt[1,2], Christian Huck[1], Bettina Frank[3], Xinghui Yin[3], Frank Neubrech[1,3], Harald Giessen[3], and Annemarie Pucci[1,2] — [1]Kirchhoff Institute for Physics, Im Neuenheimer Feld 227, Heidelberg, Germany — [2]InnovationLab GmbH, Speyerer Str. 4, Heidelberg, Germany — [3]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, Stuttgart, Germany

Electrochemically grown monocrystalline gold triangles that can be produced easily at low costs are beneficial substrates for surface-enhanced infrared absorption (SEIRA) spectroscopy as we have proven for vibrational modes of a self-assembled monolayer of octadecanethiol. Moreover, their SEIRA performance exceeds that of polycrystalline, electron beam lithographic (EBL) triangles. Produced planar but randomly orientated on a substrate, the plasmonic resonances of the monocrystalline triangles can be spectrally tuned via their edge length. It might be interesting for applications that the plasmonic response and the SEIRA signals are almost independent on the light polarization under normal incidence, which is related to the equilateral triangular shape. However, because polarization dependent resonances of linear antennas are expected to deliver stronger SEIRA enhancement, such structures were cut out from the monocrystalline platelets by means of focused ion beam. Also for the linear antennas the monocrystalline ones show a clearly stronger vibrational signal enhancement in comparison to the EBL fabricated counterparts.

O 33.4 Tue 11:15 H4

Towards Resonant Plasmonic Antenna-Enhanced Terahertz Spectroscopy — •Ksenia Weber[1], Frank Neubrech[1], Mario Hentschel[1], Michael Scherer[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart — [2]InnovationLab GmbH, Heidelberg, Germany

Terahertz spectroscopy is a technique with the potential for a vast range of sensing applications based on material-specific absorption features of molecular vibrations. However, the low absorption cross section of these excitations strongly limits its sensitivity. The possibility to increase the sensitivity of spectroscopic methods via the enhanced electromagnetic near fields provided by plasmonic nanoantennas has been shown before for surface-enhanced infrared spectroscopy (SEIRA). Our goal is to transfer the concept of SEIRA to terahertz frequencies. Here, we take a first step towards resonant antenna-enhanced terahertz spectroscopy by using plasmonic nanoantennas for the enhancement of molecular vibrations with frequencies towards the terahertz regime. We therefore fabricated arrays of rectangular gold antennas by electron beam lithography and coated them with a 30 nm thick layer of the fullerenes C60 and C70, respectively. The resonances of the structures were tailored to match the molecular vibrations located around 16 THz. The samples were investigated with Fourier transform infrared spectroscopy using a bolometer as detector. Compared to reference measurements with a pure molecular layer, an enhancement factor of four orders of magnitude is found. Our technique is a first step towards plasmon-enhanced terahertz sensing with unprecedented sensitivities.

O 33.5 Tue 11:30 H4

Investigating diffractive coupling of fs-laser induced standing gold antennas for surface enhanced IR spectroscopy — •Ruslan Röhrich[1], Tobias W. W. Mass[1], Martin Reininghaus[2], Reinhart Poprawe[2], and Thomas Taubner[1] — [1]Institute of Physics (IA) RWTH Aachen — [2]Fraunhofer Institute for Laser Technology ILT

IR resonant metallic nanoantennas induce enhanced and strongly localized electromagnetic fields. These nearfield enhancements are exploited in surface enhanced infrared absorption (SEIRA) spectroscopy to detect smallest quantities of molecules.

In this work micrometer-sized upright standing gold antennas are fabricated by irradiating a thin gold film with single femtosecond laser-pulses [1]. Due to image charge formation in the surrounding gold film, the resonance wavelength of the antennas is proportional to 4 times the antenna length [2]. The hot spot of the structure is distant from the substrate which is beneficial for SEIRA applications compared to other geometries.

By arranging these antennas in arrays, coupling between multiple antennas occurs. Collective resonances can be used to achieve stronger nearfield enhancements [3]. FTIR measurements in grazing incidence geometry and simulations demonstrate that diffractive coupling plays a significant role in the spectral response of standing antenna arrays.
[1] Wortmann et al., J. Laser Appl. **24**, 042017 (2012)
[2] Reininghaus et al., Opt. Express **21**, 32176-32183 (2013)
[3] Adato et al., PNAS **106**, 19227-19232 (2009)

O 33.6 Tue 11:45 H4

Surface-enhanced infrared spectroscopy for poly-peptide sensing on single nanostructures — •Rostyslav Semenyshyn[1], Frank Neubrech[1], Mario Hentschel[1], Xinghui Yin[1], Jochen Vogt[2], Felix Weiher[1], Christoph Stanglmair[3], Claudia Pacholski[3], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart — [2]Kirchhoff Institute for Physics, University of Heidelberg — [3]Max Planck Institute for Intelligent Systems, Stuttgart

Metal nanowires and nanoslits with plasmon resonances tuned to the infrared spectral region are ideally suited for surface enhanced infrared absorption (SEIRA) spectroscopy. Since its discovery, SEIRA has been applied to chemical analysis and biochemical sensing.

In our present work, we will demonstrate how SEIRA is used for the detection of peptides and proteins in minute amounts, and sensing of temperature-induced structural changes. For this purpose, nanostructures were functionalized by mercaptoundecanoic acid in order to selectively bind poly-L-lysine to the gold surface. Additionally, we covered other nanoantennas with specially designed collagen peptides. The plasmonic resonances of such nanostructures were tuned to the amide I and II bands of the respective poly-peptides. A tailored flow cell was used to allow the control of molecular adsorption on the nanostructures and in-situ SEIRA in aqueous solutions. Following this approach, the spectroscopic detection of about 13000 poly-peptides on one single slit could be achieved. In further experiments, structural changes of the poly-peptides due to temperature changes were observed.

O 33.7 Tue 12:00 H4

Ultrafast Vibrational Ladder Climbing on a Surface with 2D ATR IR Spectroscopy — •Jan Philip Kraack and Peter Hamm — Department of Chemistry, University of Zürich, Winterthurerstrasse 190, CH-8057

Vibrational dynamics of molecules at solid-liquid and solid-gas interfaces are important for various technical and scientific applications. In order to directly obtain multi-dimensional infrared (IR) spectra of adorbats at surfaces we have recently developed 2D Attenuated Total Reflection (ATR) IR spectroscopy.(1,2) Surface-enhancement effects in 2D ATR IR spectroscopy, stemming from plasmonic nano-structured noble-metal surfaces, have recently been characterized.(3) Here, we demonstrate optimized surface-enhancement for organic molecules on ultrathin (nm) metal surfaces which allows for vibrational ladder climbing (LC) in the electronic ground state potential of IR labels with even low extinction coefficients (< 200 M-1 cm-1). LC in such samples enables the characterization of ultrafast vibrational relaxation within the electronic ground state potential of a broad range of chemical bonds and is likely to be exploitable in coherent control(4) of surface-reactions.

(1) J.P. Kraack, D. Lotti and P. Hamm, J. Phys. Chem. Lett., 2014, 5, 2325-2329.

(2) J.P. Kraack, D. Lotti and P. Hamm, J. Chem. Phys., 2015, 142, 212413.

(3) J.P. Kraack and P. Hamm, submitted, 2015.

(4) T. Witte et al., J. Chem. Phys., 2003, 118, 2021-2024.

O 33.8 Tue 12:15 H4

Surface Phonon Polariton Localization in SiC Nano Pillars Probed by Second Harmonic Spectroscopy — •Alexander Paarmann[1], Ilya Razdolski[1], Joshua D. Caldwell[2], Alexander J. Giles[2], Sandy Gewinner[1], Wieland Schöllkopf[1], Stefan A. Maier[3], and Martin Wolf[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Navy Research Laboratory, Washington D.C., USA — [3]Imperial College, London, UK

Surface Phonon Polaritons (SPhP) have recently emerged as novel building block for mid-infrared nanophotonics, promising to possibly overcome the intrinsic loss problem of plasmonics associated with the short life time of plasmonic excitations [1]. SPhPs arise in polar dielectrics from optical phonon resonances causing negative permittivity between transversal and longitudinal optical phonon frequencies. Specifically, the long life times of optical phonons allow for remarkable degrees of SPhP localization in sub-wavelength nanostructures.

Here, we show that mid-infrared second harmonic generation (SHG) spectroscopy [2] provides the most direct experimental approach to study SPhP field localization. Our experiments employ intense, tunable, and narrowband mid-infrared pulses from a free-electron laser to acquire SHG excitation spectra from SiC nanopillars. We observe sharp enhancement of the SHG yield for various resonant modes of our nanostructures. Most importantly, the measurements show much increased sensitivity of the SHG yield to field localization, as compared to linear optical approaches. [1] Caldwell et al., Nanophotonics 4, 1 (2015), [2] Paarmann et al., APL 107, 081101 (2015)

O 33.9 Tue 12:30 H4

Second Harmonic Phonon Spectroscopy of α-Quartz — •Christopher Winta, Sandy Gewinner, Wieland Schöllkopf, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der Max-Planck-Gesellschaft

We experimentally study the efficiency of second harmonic generation (SHG) from optical phonon resonances in crystalline α-quartz, employing intense, tunable picosecond mid-infrared laser pulses generated from the FHI free-electron laser (FEL). Due to its numerous optical phonon branches, α-quartz exhibits multiple Reststrahl bands with high reflectivity, located between the respective transversal and longitudinal optical phonon resonances. For each of these spectral regions, the real part of the dielectric function is negative, resulting in rapidly attenuated evanescent waves which make these experiments sensitive to a thin near-surface layer.

In our experiments, we employ a non-collinear, reflective geometry which allows for a background-free detection of the SHG signal, even for strongly absorbing samples. Making use of the large tuning range of the FEL, we can investigate essentially all optical phonon resonances of α-quartz. We observe sharp resonances in the SHG at the frequencies of transverse optical phonons due to a resonant enhancement of the nonlinear susceptibility. At each resonance, the SHG signal also strongly depends on the azimuthal orientation of the crystal as a consequence of its trigonal crystal symmetry. We show that this feature can be exploited to selectively investigate the different contributions of the nonlinear susceptibility tensor to the SHG signal.

O 33.10 Tue 12:45 H4

Phonon control in a 2D phononic crystals — •Yuning Guo and Thomas Dekorsy — Department of Physics and Center of Applied

Photonics, University of Konstanz, 78457 Konstanz, Germany

Due to the ability to confine and mold acoustic waves in periodic nanostructure, the acoustic properties of phononic crystal (PnC) are tailored by designing various kinds of defects, which is suitable for a wide range of applications from transducer technology to filtering and guidance of acoustic waves. The ways of control phonons in 2D PnC are studied in this report. Channel drop filters can access one channel of a wavelength division multiplexed signal while leaving other channels undisturbed, which are essential components of acoustic communication systems. The target dropping frequency is selected and the transmission efficiency is improved by designing different waveguides and a series of cavities in PnC. The self-collimation of acoustic wave can be regarded as a kind of channelless phononic waveguide, which provides another way to control the propagation of phonons. The self-collimation beam can propagate with almost no diffraction along the PnC, which can be used to acoustic imaging, negative refraction etc.. When the self-collimation beam propagates in a PnC with certain defects, those defects behave like mirrors which lead to acoustic wave bending, splitting and phonons trapping. By analyzing the equi-frequency contour, the properties of waves propagating are deduced and the frequency of self-collimation is determined.

O 33.11 Tue 13:00 H4

Large-Area Fabrication of TiN Nanoantenna Arrays for Refractory Plasmonics in the Mid-Infrared. — •Shahin Bagheri[1], Christine M. Zgrabik[2], Timo Gissibl[1], Andreas Tittl[1], Florian Sterl[1], Ramon Walter[1], Stefano De Zuani[3], Audrey Berrier[3], Thomas Stauden[4], Gunther Richter[5], Evelyn L. Hu[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, Stuttgart, Germany. — [2]School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA. — [3]1st Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, Stuttgart, Germany. — [4]Fachgebiet Nanotechnologie, Technische Universität Ilmenau, Ilmenau, Germany. — [5]Max-Planck-Institut für Intelligente Systeme, D-70589 Stuttgart, Germany.

We utilize fast and wafer-scale fabrication methods such as direct laser writing and laser interference lithography to fabricate large-area nanoantenna arrays of TiN. Our lithographic tools allow for fast and homogeneous preparation of nanoantenna geometries on a polymer layer, which is then selectively transferred to TiN by subsequent argon ion beam and chemical wet etching process. Tailoring of the TiN antenna geometry enables precise tuning of the plasmon resonances from the near to the mid-infrared spectral range. The antennas are protected by an additional Al2O3 layer which allows for high-temperature annealing in argon flow without loss of the plasmonic properties.

O 33.12 Tue 13:15 H4

Resonances from thermal waves using photothermal deflection microscopy — •André Heber, Markus Selmke, and Frank Cichos — Universität Leipzig, Exp. Phys. I, Molecular Nano-Photonics Group, 04103 Leipzig, Germany

A gold nanoparticle is heated by a harmonically modulated pump laser which is fixed in space. This configuration results in a thermal wave centred around the nanoparticle. The thermal wave is exponentially damped with a decay-length corresponding to a single thermal wavelength. We co-align a second laser beam which is non-absorbed and steerable to measure deflections induced by refractive index changes due to the optical heating. This setup enables the detection of the thermal wave's resonances in the components in phase and out-of-phase with the pump. The deflection signal depends on the distance. The externally controllable offset provides a well-defined length scale which can be used to quantify the thermal diffusivities from these resonances in combination with a ray optics model.

O 34: Nanostructures at Surfaces II

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

O 34.1 Tue 10:30 H6

Hydrogen-bonded bimolecular network on Au(111) — •Christian Steiner[1], Zechao Yang[1], Ute Meinhardt[2], Bettina Gliemann[2], Martin Gurrath[3], Bernd Meyer[3], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, FAU Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg, Germany — [3]Computer-Chemie-Centrum, FAU Erlangen-Nürnberg, Germany

Understanding and controlling the formation of multi-component molecular self-assemblies is important for the design of donor-acceptor networks which are an integral part of organic optoelectronic devices. We discuss the self-assembly and electronic properties of monomolecular[1] and bimolecular networks assembled from carboxyl- and diaminotriazinyl-functionalized triphenylamine derivatives based on low-temperature scanning tunneling microscopy experiments and density functional theory calculations. On Au(111), both molecules arrange in large porous hydrogen-bonded networks in order to optimize the intermolecular hydrogen bonding. Upon co-adsorption, the molecules form perfectly ordered bimolecular honeycomb networks stabilized by bonds between the carboxyl and the diaminotriazinyl groups. The HOMO-LUMO gap in the mixed network is defined by the two types of molecules, which is typical for an electron donor-acceptor scheme.

[1] C. Steiner et al. J. Phys. Chem. C, 119 (46), 25945-25955 (2015)

O 34.2 Tue 10:45 H6

Self-assembling and chemistry of ferrocene dicarboxylic acid on different substrates — •Jan Berger[1], Olexandr Stetsovych[1], Krzysztof Kośmider[1], Martin Vondráček[2], Martin Švec[1], and Pavel Jelínek[1] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, CZ-16200, Prague, Czech Republic — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 1999/2, CZ-18221, Prague, Czech Republic

Ferrocene based molecules are extremely appealing as they provide the possibility of having built-in spin or charge functionalities. However there are only limited studies of structural and electronic properties on surfaces so far. We investigated self-assembling processes of ferrocene-based molecules on both metallic (Ag(111), Cu(110)) and insulating (Cu3N/Cu(110)) with high-resolution AFM/STM combined with XPS and NEXAFS. The experimental evidence is corroborated with total energy DFT calculations and advanced AFM simulations. The analysis of the data allows understanding of the unique arrangement and adsorption geometry of the molecules on each substrate, as well as the chemical changes of the carboxylic groups. Where the molecules on the Ag(111) show only a weak interaction with the substrate and a complex self-assembling configuration. On the Cu(110) and Cu3N/Cu(110) the carboxylic groups are a subject to dehydrogenation forming strong chemical bond to the substrate onto the Cu atoms, keeping an upright orientation of the ferrocene cyclopentadienide rings.

O 34.3 Tue 11:00 H6

On-surface synthesis of covalent organic nanostructures on metals and strategies for post synthetic decoupling — •Atena Rastgoo Lahrood[1,2], Jonas Björk[3], Matthias Lischka[1,2], Johanna Eichhorn[1,2], Wolfgang M. Heckl[1,2,4], and Markus Lackinger[1,2,4] — [1]Department of Physics, Tech. Univ. Munich, James-Franck-Str. 1, 85748 Garching — [2]Center for NanoScience (CeNS), Schellingstr. 4, 80799 Munich — [3]Department of Physics Chemistry and Biology, IFM Linköping University, 58183 Linköping, Sweden — [4]Deutsches Museum, Museumsinsel 1, 80538 Munich

On-surface polymerization is a versatile approach for the synthesis of otherwise inaccessible extended low-dimensional organic nanostructures. Ullmann coupling as the most favored reaction relies on the reactivity of metal surfaces to initiate the coupling by dissociating halogen substituents. Since the metal surfaces that are indispensable for the synthesis are unfavorable for many applications, we explore strategies for a post synthetic detachment.

Surface chemical studies of 1,3-diiodobenzene on Cu(111) revealed covalently coupled trimers as reaction products adsorbed atop a closed iodine monolayer rather than directly on the metal surface. These unexpected results suggest iodine adsorbs underneath the organics, thereby indicating possibilities for using iodine monolayers for post_synthetic decoupling.

This approach was verified by exposing on-surface synthesized covalent porous 2D polyphenylene networks to iodine vapor. Samples were characterized by STM, XPS, and NEXAFS.

O 34.4 Tue 11:15 H6

On-surface synthesis of non-symmetric molecular nodes — •Christophe Nacci[1], Francisco Ample[2], Andreas Viertel[3], Stefan Hecht[4], Christian Joachim[5], and Leonhard Grill[6] — [1]Department of Physical Chemistry, University of Graz, Austria — [2]IMRE, Singapore — [3]Department of Chemistry, Humboldt-Universität zu Berlin, Germany — [4]Department of Chemistry, Humboldt-Universität zu Berlin, Germany — [5]CEMES-CNRS, Toulouse, France — [6]Department of Physical Chemistry, University of Graz, Austria

On-surface synthesis is a promising strategy for building complex molecular architectures that are potentially relevant in the field of molecular electronics. Suitable design of molecular building blocks is required in order to assemble functional molecules into stable covalently bound networks with a well-defined spatial arrangement. In this presentation low-temperature scanning tunneling microscopy and spectroscopy are used to image individual molecules and determine their electronic properties at surface with high spatial resolution. Non-symmetric molecular nodes comprised of central molecule and equipped with short polyfluorene wires at predefined positions were grown by on-surface synthesis. The asymmetric node structure is highly desired since it encodes different conjugated pathways, i.e. potentially different electrical channels. The assembly of different molecular nodes will be discussed as well as the electrical characterization of individual non-symmetric molecular nodes by pulling them off a supporting surface with the tip of a scanning tunneling microscope.

O 34.5 Tue 11:30 H6

Interplay of chemical and electronic structure on the single-molecule level in 2D polymerization — •Claudius Morchutt[1,3], Jonas Björk[2], Carola Strasser[3], Ulrich Starke[3], Rico Gutzler[3], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Department of Physics, Chemistry and Biology, IFM, Linköping University, 58183 Linköping, Sweden — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Single-layers of covalently-linked organic materials in the form of two-dimensional (2D) polymers constitute structures complementary to inorganic 2D materials. The electronic properties of the 2D polymer can be manipulated through a deliberate choice of precursor organic molecules. In this work, the changes in electronic structure from precursor molecule to oligomer are addressed by scanning tunneling spectroscopy and ultra violet photoelectron spectroscopy. The polymerization reaction of 1,3,5-tris(4-carboxyphenyl)benzene via reductive decarboxylation on Cu(111) is investigated by scanning tunneling microscopy, x-ray photoelectron spectroscopy and density functional theory calculations. We present a comprehensive study of an on-surface coupling reaction without contaminating side-products and we show HOMO/LUMO shifts as a consequence of decarboxylation and polymerization on the molecular level.

O 34.6 Tue 11:45 H6

Templated bilayer self-assembly of fully conjugated π-expanded macrocyclic oligothiophenes complexed with fullerenes — •Jose D. Cojal Gonzalez[1], Masahiko Iyoda[2], and Jürgen P. Rabe[1] — [1]Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin — [2]Department of Chemistry, Graduate School of Science and Engineering, Tokyo Metropolitan University, Hachioji, Tokyo

Fully conjugated π-expanded macrocyclic oligothiophenes have been envisaged for host-guest systems, as building blocks for supramolecular nanostructures and photovoltaic applications due to their structural, optical and electronic properties. However, control over the self-assembly of such systems still remains a challenge. Here, we report a self-assembled monolayer of hydrogen-bonded trimesic acid at the interface between its heptanoic acid solution and highly oriented pyrolytic graphite. This monolayer is shown to provide host-sites for the epitaxial ordering of Saturn-like complexes of fullerenes with π-expanded oligothiophene macrocycles(1) in mono- and bilayers. The bilayer and triple layer formation was confirmed by STM tomography, based on discrete bias set-point imaging of each layer. All force-field potential interaction energy calculations confirmed the stability of the multilayer architecture. Finally, Scanning Tunneling Spectroscopy (STS) of the layers allowed for determination of the rectification characteristics and the position of the combined frontier orbitals.

(1) Shimizu H, Cojal Gonzalez JD, Hasegawa M, Nishinaga T, Haque T, Takase M, Otani H, Rabe JP and Iyoda M 2015 *J. Am. Chem. Soc.* **137**, 3877-3885

O 34.7 Tue 12:00 H6

A comparative study of two perylene derivatives on Cu(111): insight into the bonding mechanism — •Mihaela Enache[1], Manfred Matena[2], Jonas Björk[3], Jorge Lobo-Checa[4], Thomas Jung[2], Mats Persson[5], and Lutz Gade[6] — [1]University of Groningen, Groningen, Netherlands — [2]University of Basel, Basel, Switzerland — [3]University of Linköping, Linköping, Sweden — [4]Centro de Física de Materiales (CSIC-UPV-EHU), San Sebastian, Spain — [5]University of Liverpool, Liverpool, UK — [6]Universität Heidelberg, Heidelberg, Germany

Herein, an experimental and theoretical characterization of the adsorption of two perylene derivatives on Cu(111) is presented [1, 2]. The main focus of this work lies on the analysis of molecule-molecule and molecule-substrate interactions by combining results from scanning tunneling microscopy, x-ray photoelectron spectroscopy, x-ray standing wave (XSW) measurements, and density functional theory.

For submonolayer coverage and after annealing (>150°C), both systems form a metal-coordinated network, which is commensurate to the substrate. By performing XSW measurements, the vertical adsorption geometry was determined and thereby, insight into the interplay between intermolecular and molecule-substrate interactions was gained. As a result of the metal coordination, the molecule-substrate interactions are decreased and the molecules are essentially decoupled from the Cu(111) surface.

[1] M. Matena et al., Phys. Rev. B, 90, 125408 (2014)
[2] M. Matena et al., Chem. Eur. J., 16, 2079 (2010)

O 34.8 Tue 12:15 H6

On-surface fabrication of acenes — •Justus Krüger[1], Niko Pavliček[2], Frank Eisenhut[1], José M. Alonso[3], Dolores Pérez[3], Enrique Guitián[3], Thomas Lehmann[2], Dmitry Ryndyk[2], André Gourdon[4], Gerhard Meyer[2], Leo Gross[2], Diego Peña[3], Gianaurelio Cuniberti[1], and Francesca Moresco[1] — [1]Institute for Materials Science, Max Bergmann Center of Biomaterials, and Center for Advancing Electronics Dresden, TU Dresden, 01069 Dresden, Germany — [2]IBM Research-Zurich, 8803 Rüschlikon, Switzerland — [3]CIQUS and Departamento de Química Orgánica, Universidade de Santiago de Compostela. Santiago de Compostela 15782, Spain — [4]CEMES, UPR 8011 CNRS, Nanosciences Group, 29 Rue J. Marvig, P.O. Box 94347, 31055 Toulouse, France

We present the on-surface reduction of acene-derivatives to form genuine acenes (hydrocarbons with linearly fused benzene rings) on Au(111) and Cu(111). The conversion is achieved by scanning tunneling microscopy (STM) tip-induced manipulation as well as thermal activation and is conclusively demonstrated by means of atomic force microscopy with atomic resolution. This observed transformation may pave the way for the on-surface preparation and stabilization of even higher acenes.

O 35: Ultrafast Phenomena I

Time: Tuesday 9:30–13:15 Location: H10

O 35.1 Tue 9:30 H10

Sub-cycle quantum interference in solid-state high-harmonic generation — •Matthias Hohenleutner[1], Fabian Langer[1], Olaf Schubert[1], Matthias Knorr[1], Christoph Lange[1], Ulrich Huttner[2], Stephan W. Koch[2], Mackillo Kira[2], and Rupert Huber[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]University of Marburg, 35032 Marburg, Germany

Utilizing intense light pulses to control electron motion in atoms and molecules has opened up spectacular new routes in ultrafast and attosecond photonics such as high-harmonic generation (HHG). The recent discovery of HHG in solids combines ultrafast quantum control with complex condensed matter systems. We employ intense, phase-controlled multi-THz waveforms to drive HHG in bulk gallium selenide. Non-resonantly driven interband polarization and simultaneous intraband carrier acceleration throughout the entire Brillouin zone result in the emission of extremely broadband, phase-locked high-harmonics (HH). More importantly yet, sub-cycle time- and field-resolution allows us to directly trace the underlying electron dynamics with precise temporal correlation to the driving waveform. Remarkably, the HH are emitted as a unipolar train of ultrashort, nearly unchirped few-femtosecond bursts, which coincide precisely with the driving field maxima. These features unravel a novel quantum interference of multiple interband excitation paths during HHG, as explained by our microscopic quantum theory. The first direct time domain study of HH from solids paves the way towards a full quantum picture of the underlying mechanisms and sparks hope for solid-state sub-femtosecond sources.

O 35.2 Tue 9:45 H10

Lattice dynamics of optically excited few-layer graphite — Christian Gerbig, Silvio Morgenstern, Marlene Adrian, Cristian Sarpe, •Arne Senftleben, and Thomas Baumert — Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel

Time-resolved diffraction with femtosecond electron pulses has become a promising technique to directly provide insights into photo induced primary dynamics at the atomic level in molecules and solids. Ultrashort pulse duration as well as extensive spatial coherence are desired, however, space charge effects complicate the bunching of multiple electrons in a single pulse. We experimentally investigate the interplay between spatial and temporal aspects of resolution limits in ultrafast electron diffraction (UED) on our highly compact transmission electron diffractometer. To that end, the initial source size and charge density of electron bunches are systematically manipulated and the resulting bunch properties at the sample position are fully characterized in terms of lateral coherence, temporal width and diffracted intensity. We obtain electron pulse durations down to 120 fs and transversal coherence lengths up to 20 nm. Instrumental impacts on the effective signal yield in diffraction and electron pulse brightness are discussed as well. The performance of our compact UED setup at selected electron pulse conditions is finally demonstrated in a time-resolved study of lattice heating in few-layer graphite after optical excitation. During the heating process, we observe shearing modes and acoustic breathing modes.

O 35.3 Tue 10:00 H10

Ultrafast carrier dynamics in bulk MoS_2 studied by transient absorption spectroscopy — •Tim Völzer, Matthias Lütgens, Franziska Fennel, and Stefan Lochbrunner — Institut für Physik, Universität Rostock, Albert-Einstein-Str. 23, 18059 Rostock

Transistion metal dichalcogenides feature unique electronic and optical properties. In addition, they are characterised by a layered structure, allowing the preparation of atomically thin crystals. As a representative of those materials, molybdenum disulfide is suggested as a promising candidate for optoelectronic and photocatalytic applications. To characterise the optical excitation and its dynamics we performed both static transmission and time-resolved pump-probe spectroscopy.

Two absorption bands, labelled A and B, are observed in the static absorption spectrum which are attributed to direct transitions at the K point of the Brillouin zone. The lower electronic transition is excited within the femtosecond absorption measurements and the dynamics is followed by a white light continuum covering the whole visible range. A decrease of absorption for the A and B transition is observed whereas an increase of absorption is present for lower energies. This signature is indicative for a band renormalization induced by the population in the first excited band. The subsequent signal decay shows two distinct time dependencies, an exponential sub picosecond contribution caused by carrier-carrier and carrier-phonon scattering and a strongly non-exponential component for longer times. The latter is attributed to electron-hole recombination via defect states and shows an acceleration with increasing excitation density.

O 35.4 Tue 10:15 H10

Internal structure and ultrafast dynamics of excitons in monolayer WSe_2 — •Christoph Pöllmann[1], Philipp Steinleitner[1], Ursula Leierseder[1], Philipp Nagler[1], Gerd Plechinger[1], Michael Porer[1], Rudolph Bratschitsch[2], Christian Schüller[1], Tobias Korn[1], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Physics, University of Münster, 48149 Münster, Germany

Atomically thin transition metal dichalcogenides (TMDCs) promise groundbreaking optoelectronic applications and devices due to their direct bandgap in the optical range. As a consequence of the layered structure, unusually strongly bound excitons can exist even at room temperature, dominating the optical and electronical properties. In order to exploit the full potential of this new material system, key open questions regarding the excitons in TMDC monolayers have to be answered. Here we report the first direct observation of the intraexcitonic 1s-2p transition via time resolved pump/THz probe studies, tracing both optically bright and dark exciton states. Beside quantitative information about transition energies, oscillator strengths, linewidths and many-body effects a record fast radiative decay of bright excitons with a time constant of only 150 fs can be revealed.

O 35.5 Tue 10:30 H10

Auger Recombination and Charge Transfer of CdSe/CdS Core/Shell Quantum Dot/Quantum Rods — •Mona Rafipoor[1,2], Jan Niehaus[3], Holger Lange[1,2], and Horst Weller[1,2,3] — [1]Universität Hamburg, Institut für Physikalische Chemie, Grindelallee 117, 20146 Hamburg — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]CAN GmbH Grindelallee 117 20146 Hamburg

We investigated clustered CdSe/CdS quantum dots/quantum rods (QDQRs) by time-resolved optical spectroscopy.

Power dependent measurements were conducted by excitation with different intensities and recording time traces of the photoluminescence (PL) decay simultaneously with the PL intensity. Increasing the excitation power generally increases the average exciton population per QDQR. We observe signatures of exciton-exciton interactions starting with exciton populations of one. This is tentatively assigned to an interaction between the excitons across the QDQRs. The non-monotonic increase of the PL intensity with excitation power in this regime supports the idea of a new, non-radiative multiexciton decay across the cluster.

To get more Information about this kind of interaction we apply Transient Absorption spectroscopy. By varying the pump wavelength, we are able to specifically excite core and shell and follow the subsequent relaxation.

O 35.6 Tue 10:45 H10

The role of intervalley scattering and phonon softening in the ultrafast carrier dynamics of PbTe — Prashant Padmanabhan, Kestutis Budzinauskas, Kiran H. Prabhakara, and •Paul H. M. van Loosdrecht — Physics Institute 2, University of Cologne, 50937 Cologne, Germany

PbTe is a leading thermoelectric material, notable for its low thermal conductivity and unusually large carrier mobility at very low doping levels. Here, we report on ultrafast pump-probe experiments on PbTe that shed light on the ultrafast relaxation of highly excited carriers. By employing time-resolved differential reflectivity measurements, we probe the dynamics of electron-electron and electron-phonon interactions on the femtosecond time-scale. Additionally, the use of a super-continuum probe pulse allows us to investigate the wavelength dependence of the carrier relaxation dynamics. Our results suggest that phonon mediated intervalley scattering involving the band gap between the Γ and K points plays a significant role in carrier cooling. Further, the temperature dependence of these dynamics point to anomalous behavior that may be the result of phonon softening, recently reported to be a key element in the unique thermal properties of PbTe.

O 35.7 Tue 11:00 H10

Theory of the coherent A$_{1g}$ phonon decay in antimony — •Sergej Krylow, Eeuwe S. Zijlstra, and Martin E. Garcia — Universität Kassel, Theoretische Physik II, Heinrich-Plett-Straße 40, 34132 Kassel,Germany

The fluence-dependent decay paths of the femtosecond laser-excited coherent A$_{1g}$ phonon mode in antimony are investigated by means of electronic-temperature-dependent density-functional-theory molecular-dynamics simulations, which yield an exponentially decaying coherent phonon, comparable to experiments. Additional calculations of the phonon dispersion indicate that third order decay processes occur mainly within the acoustic and fourth order processes within the optical phonon branches. This can also be seen in the subsequent analysis of the molecular dynamics simulations, which reveal that the third and fourth order phonon contributions to the decay can be influenced by means of the applied fluence.

30 min. Coffee Break

Invited Talk O 35.8 Tue 11:45 H10

Coherent Quantum Dynamics of Excitons in Atomically Thin Semiconductors — •xiaoqin li — Univ. of Texas-Austin, Austin, USA

The transitional metal dichalcogenides (TMDs) are an emerging class of atomically thin semiconductors with tightly-bound excitons and charged excitons (i.e. trions). A fundamental property of these quasiparticles is quantum decoherence time, which reflects irreversible quantum dissipation arising from system (excitons) and bath (vacuum and other quasiparticles) interaction and determines the timescale during which excitons can be coherently manipulated. Dephasing time is also equivalent to the intrinsic homogeneous linewidth of exciton resonances. In addition, excitons in TMDs are localized at the corners of the Brillouin zone and provide a convenient way to optically manipulate the valley degree of freedom. Direct measurement of valley coherence time is challenging because it corresponds to nonradiative coherence between two degenerate states. Using ultrafast multi-dimensional optical spectroscopy, we investigate the intrinsic homogeneous linewidth of excitons, exciton valley coherence as well as coupling between excitons and trions. Our studies reveal coherent exciton dynamics on the order of ~ 100 fs in monolayer TMDs. Decoherence time is not only an important parameter for characterizing fundamental properties of excitons, but also serves as a sensitive probe for exciton-exciton and exciton-phonon interaction.

O 35.9 Tue 12:15 H10

Ultrafast Pump-Probe Analysis of Exciton-Polariton Propagation — Jan Lohrenz^{1}, Stephan Melzer^{1}, Claudia Ruppert^{1}, Ilya Akimov^{1}, •Matthias Reichelt^{2}, Alexander Trautmann^{2}, Torsten Meier^{2}, and Markus Betz^{1} — ^{1}Experimentelle Physik 2, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — ^{2}Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

In bulk CdZnTe light is significantly slowed down in a spectral range close to the lower exciton-polariton branch. [1] Here, we investigate nonlinear optical signatures in a pump-probe experiment with femtosecond laser pulses. Experimental data and model simulations for the optical response of a nonlinearly driven two-level system suggest that the excitation induced dephasing [2] and slow light propagation lead to unexpected features in the differential transmission spectra. [3]

[1] T. Godde, I. A. Akimov, D. R. Yakovlev, H. Mariette, and M. Bayer, Phys. Rev. B **82**, 115332 (2010).

[2] H. Wang, K. Ferrio, D.G. Steel, Y.Z. Hu, R. Binder, and S.W. Koch, Phys. Rev. Lett. **71**, 1261 (1993).

[3] J. Lohrenz, S. Melzer, C. Ruppert, I.A. Akimov, M. Reichelt, A. Trautmann, T. Meier, M. Betz, to be published.

O 35.10 Tue 12:30 H10

Dynamics of exciton-polariton condensates in semiconductor microcavities with periodic potentials — •Xuekai Ma^{1}, Stefan Schumacher^{1}, and Oleg Egorov^{2} — ^{1}Physics Department, Universität Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany — ^{2}Institute of Condensed Matter Theory and Solid State Optics, Abbe Center of Photonics, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Exciton-polaritons are quasi-particles made of quantum well (QW) excitons coupled to cavity photons. They have very small effective mass ($10^{-4} m_e$) and lifetimes on the tens of picoseconds scale. Due to their photonic properties, they can be excited by light and probed, respectively. Due to their excitonic properties, nonlinearity is introduced into this system at elevated densities. Polaritons, which are composite bosons, can undergo a condensation process (with similarities to Bose-Einstein condensation) under incoherent excitation. Many features in the dynamics of polariton condensates can be described by a modified Gross-Piteavskii equation (GPE). Here, we study the nonlinear dynamics of polariton condensates in periodic potentials. In the presence of a periodic potential, a band structure including a band-gap can be obtained. We show that polariton condensates can occupy and switch between different energy states by changing the pump excitation intensity and shape. Our simulation results agree very well with recent experimental results.

O 35.11 Tue 12:45 H10

Nonlinear terahertz quantum control of Landau-quantized electrons — •Thomas Maag^{1}, Andreas Bayer^{1}, Sebastian Baierl^{1}, Matthias Hohenleutner^{1}, Tobias Korn^{1}, Christian Schüller^{1}, Dominique Bougeard^{1}, Christoph Lange^{1}, Rupert Huber^{1}, Martin Mootz^{2}, Stephan W. Koch^{2}, and Mackillo Kira^{2} — ^{1}Department of Physics, University of Regensburg, 93053 Regensburg, Germany — ^{2}Department of Physics, Philipps-University Marburg, 35032 Marburg, Germany

Controlling superpositions of many-body electronic quantum states in solids is impeded by rapid dephasing through inter-particle scattering. However, Walter Kohn found in 1961 that the cyclotron resonance of Landau-quantized electrons in a two-dimensional electron gas (2DEG) is immune to Coulomb forces. This protection warrants long coherence times and makes the system interesting for quantum control, but explicitly excludes nonlinearities. Here, we demonstrate how intense light pulses in the terahertz (THz) spectral range can induce well-controlled electronic many-body correlations in a magnetically biased 2DEG and tailor a distinctly anharmonic response. Coherent ladder climbing up to the 6th rung yields population inversion and abruptly increases dephasing. Strikingly, 2D THz spectroscopy reveals distinct multi-wave mixing signatures, which our quantum theory explains through Coulomb interactions between electrons and the positively charged ionic background. These many-body dynamics demonstrate how internal degrees of freedom of solid state quantum systems enable coherent nonlinear interactions for future ultrafast quantum information processing.

O 35.12 Tue 13:00 H10

Ultrafast nonlinear response of GaAs under high pressures — •Johannes M. Braun^{1,2}, Jan F. Schmidt^{3}, Denis V. Seletskiy^{3}, Harald Schneider^{1}, Manfred Helm^{1,2}, and Alexej Pashkin^{1,3} — ^{1}Helmholtz-Zentrum Dresden-Rossendorf, Germany — ^{2}TU Dresden, Germany — ^{3}Department of Physics and Center for Applied Photonics, University of Konstanz, Germany

Applying hydrostatic pressure leads to dramatic changes in the band structure of semiconductors. In particular, it enables a continuous tuning of the bandgap energy. Here we study the nonlinear response of bulk gallium arsenide (GaAs) in the vicinity of its bandgap. The optical pump-probe experiment is performed in a non-collinear reflection geometry at pressures up to 3 GPa generated inside a diamond anvil cell. By increasing pressure we observe pronounced slowing down of the relaxation dynamics of photoexcited charge carriers: the time constant of the dominating relaxation process increases from about 10 ps at ambient pressure to 35 ps above 0.7 GPa. These time scales are by an order of magnitude shorter than the recombination time determined using optical pump - THz probe spectroscopy. Thus, the fast dynamics observed in the optical pump-probe measurements is governed by the cooling of hot electron distribution and not by the recombination process. Furthermore, at pressures above 2 GPa the bandgap energy of GaAs is above the excitation spectrum of our experiment. The sample becomes transparent for the femtosecond pulses leading to a transient pump-probe signal with a negative sign due to the third order nonlinear response of GaAs.

O 36: Gaede Prize Talks

The prestigious Gaede prize of the German Vacuum Society (DVG e.V.) founded by Dr. Manfred Dunkel, head of the Leybold company for many years, is supported by Oerlikon Leybold Vacuum GmbH and regularly presented at the DPG Spring Meeting by the Surface Science and Thin Films Divisions. The Gaede prize is yearly awarded to young scientists (prior to their first professorship) for outstanding basic and applied research in the fields of vacuum physics and technology, thin films, surface science, materials and methods in solid state electronics, or nanotechnology. This symposium celebrates 30 years of Gaede prize, the first one being awarded to J. Kirschner in 1986. It comprises talks by the prize winner of this year, Dr. Julia Stähler (FHI Berlin), and previous winners, Prof. Jürgen Fassbender and Prof. Eberhard Umbach, complemented by the history of Gaede (Dr. Gerhard Voss, DVG and Head of the Vacuum Science and Technology Division of DPG). The list of previous prize winners (http://www.gaedepreis.org/preistraeger.html) comprises a large number of nowadays renowned colleagues for whom the Gaede prize was very supportive for their career.

Organizers: Dietrich R.T. Zahn (TU Chemnitz), Martin Wolf (FHI Berlin) and Norbert Esser (ISAS Berlin)

Time: Tuesday 13:30–15:30 Location: H11

Special Talk O 36.1 Tue 13:30 H11
Wolfgang Gaede - Wegbereiter der modernen Vakuum-Technik — •Gerhard Voss — Oerlikon Leybold Vacuum, Köln

In diesem Vortrag geht es nicht nur um den Lebenslauf von Wolfgang Gaede, sondern auch um einige seiner wichtigsten Erfindungen, wie die Verbesserung der rotierenden Kapsel-pumpe (= Drehschieber-Pumpe), die Molekular(luft)pumpe, die Diffusionspumpe und die Drehschieber-Pumpe mit Gas-Ballast-Einrichtung.

Die bedeutenden Erfindungen von Wolfgang Gaede haben den enormen Aufschwung der Vakuum-Technik nach dem zweiten Weltkrieg erst möglich gemacht und stehen auch heute noch im Einsatz.

Prize Talk O 36.2 Tue 14:00 H11
Ultrafast dynamics of many-body effects in solids and at interfaces: Polarons, excitons and correlated electrons — •Julia Stähler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Optical excitation of solids can lead to various interesting non-equilibrium phenomena that occur on electronic time and energy scales. These, for instance, involve the interaction of excited charge carriers among each other as well as with the lattice degrees of freedom. Key ingredient for such many-body effects is the Coulomb interaction and, importantly, its *screening*. Modification of the latter on ultrafast timescales disturbs the balance of competing forces in a system and can, thus, give rise to interesting transient properties. Exemplary for the diversity of such many-body effects and their impact also on the *equilibrium* qualities of materials, I will discuss the following three phenomena:

(i) Ultrafast dynamics of charge injection, trapping and polaronic stabilization during the birth of a solvated electron [1]

(ii) Femtosecond electron relaxation and ultrafast formation of excitons at polar and non-polar ZnO surfaces [2]

(iii) Instantaneous insulator-to-metal transition in photoexcited monoclinic VO_2 [3]

[1] J. Stähler *et al. J. Am. Chem. Soc.* **137**, 3520 (2015)
[2] J.-C. Deinert *et al. Phys. Rev. Lett.* **113**, 057602 (2014)
[3] D. Wegkamp *et al. Phys. Rev. Lett.* **113**, 216401 (2014)

Special Talk O 36.3 Tue 14:30 H11
Ion beam modification of magnetic materials - revisited — •Jürgen Fassbender — Helmholtz-Zentrum Dresden-Rossendorf

In 2009 the Gaede prize was awarded for the ion induced modification and patterning of thin magnetic films. At that time most of the investigations were dealing with the local modification of magnetic anisotropies and exchange bias phenomena. In recent years we could show that also other magnetic properties, e.g. magnetic relaxation processes [1], can be tailored, but also the ferromagnetic state itself can be created [2] or destroyed depending on the material system under investigation. In particular the latter modifications open a route to the creation of nanomagnets [3] and magnonic crystals [4] by local ion irradiation. A current review will be given.

[1] M. Körner et al., Phys. Rev. B 88, 054405 (2013).
[2] R. Bali et al., Nano Lett. 14, 435 (2014).
[3] F. Röder et al., Sci. Rep. 5, 16786 (2015).
[4] B. Obry et al., Appl. Phys. Lett. 102, 202403 (2013).

Special Talk O 36.4 Tue 15:00 H11
Large-scale reconstruction of metal-organic interfaces induced by chemisorption and surface stress change — •Eberhard Umbach[1,2], Florian Pollinger[1,3], Stefan Schmitt[1,4], Thomas Schmidt[2], Helder Marchetto[2], and Achim Schöll[1] — [1]Exp. Physik VII, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Fritz-Haber-Institut der MPG, Abt. CP, 14195 Berlin — [3]Physikalisch-Technische Bundesanstalt, D-38116 Braunschweig — [4]SPECS GmbH, D-13355 Berlin

The adsorption of large organic molecules on metal substrates can have enormous influence on the topography, geometric structure, and electronic properties of this interface provided that the interaction is chemisorptive. Thus, under certain preparation conditions large scale reconstructions may occur which originate from a significant change of surface stress and may involve large mass transport. These reconstructions can lead to regular nano-patterns which are useable as templates in a bottom-up approach in nanotechnology. More important could be that such reconstructions may have considerable influence on the electric and optical properties of metal-organic devices, and can even lead to failure, if, e.g., the interface between metallic electrode and adjacent organic layer changes under operating conditions.

The talk will address this topic using the archetype system PTCDA on various Ag surfaces some of which are highly-indexed (vicinal). Results from various surface methods including STM, spectro-microscopy and a cantilever bending method will be presented to analyze and interpret the results.

O 37: Nanostructures at Surfaces III

Time: Tuesday 14:00–16:00 Location: S054

Invited Talk O 37.1 Tue 14:00 S054
Metal Complexation of Sulfur on Coinage Metal Surfaces — •Patricia Thiel[1], Holly Walen[1], Yousoo Kim[2], Junepyo Oh[2], Hyun Jin Yang[2], and Da-Jiang Liu[3] — [1]Iowa State University, Ames, Iowa USA — [2]RIKEN Surface and Interface Science Laboratory, Wako, Saitama Japan — [3]Ames Laboratory, Ames, Iowa USA

It is well known that chemisorbed chalcogens (oxygen, sulfur, selenium) on metal surfaces can induce or lift surface reconstruction. Less well-known is the fact that they can form metal-chalcogen complexes in which the source of metal atoms is the surface itself. Chalcogens can also impact the formation of metal nanostructures during metal deposition, as well as the stability of such nanostructures. We focus on behavior for sulfur (S) on Cu, Ag, and Au surfaces at low coverage (less than 0.1 monolayer) to avoid competition from surface reconstructions, and at low temperature to ensure immobilization. Under these conditions, complex formation is prominent for (111) surfaces of Cu and Ag , where they are proposed to result in a strong destabilization of monolayer islands by providing an alternative vehicle for efficient surface mass transport. For Au(111), S lifts the herringbone reconstruction, but does not produce complexes at low coverage. From these and other studies, a common structural motif emerges: a S-M-S staple-like unit that may be the dominant mass carrier at realistic temperature.

O 37.2 Tue 14:30 S054

Bromine-functionalized pyrene derivatives on metal surfaces: self-assembly and on-surface polymerization — •Bay V. Tran[1], Tuan Anh Pham[1], Fei Song[1], Manh Thuong Nguyen[2], Milan Kivala[3], Lutz H. Gade[4], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, the Netherlands — [2]The Abdus Salam International Center for Theoretical Physics, Italy — [3]Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Germany — [4]Anorganisch-Chemisches Institut, University of Heidelberg, Germany

On-surface polymerization under ultrahigh vacuum conditions, an alternative method compared to solution-based synthesis, is considered as a promising route in the bottom-up approach for constructing novel 1D and 2D materials. One of the intriguing materials which can be reliably obtained through on-surface polymerization based on Ullmann coupling is graphene nanoribbons. On the other hand, the controlled construction of sufficiently large 2D polymer networks still represents a challenge.

In this work, we report on both the self-assembly as well as the on-surface polymerization of bromine-functionalized pyrene derivatives on Au and Cu surfaces. The experiments (combining scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS) measurements) were performed under UHV conditions. Insight was obtained with respect to the structural and electronic properties of the as-deposited molecular monomers as well as the polymer networks generated through thermal annealing.

O 37.3 Tue 14:45 S054

Properties of self-assembled molecular structures formed by triarylamine derivatives on the KBr(001) surface — •Martin Gurrath[1], Christian Steiner[2], Sabine Maier[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Department of Physics, FAU Erlangen-Nürnberg

Non-contact AFM measurements show that triarylamine molecules with different functional end and side groups form a variety of 1D, 2D and 3D molecular assemblies on a KBr(001) substrate.

Using density-functional theory calculations we analyzed the molecule–molecule and molecule–substrate interactions that lead to the different growth modes.

First, a series of gas phase calculations of dimerization energies was performed to determine the molecule–molecule interaction strength for pi-stacking and different hydrogen bonding motifs.

Then, the binding configuration and binding strength of the molecules on the KBr(001) substrate were determined by calculating the adsorption energies of single molecules and dimers.

Finally, monolayer arrangements were derived from the most favorable dimer structures.

The analysis of the different contributions to the adsorption energy allows us to rationalize why specific structures are formed by the molecules on KBr(001) and enables us to predict, how molecule–molecule and molecule–substrate interactions can be tuned in order to achieve 1D, 2D or 3D assembly of the molecules.

O 37.4 Tue 15:00 S054

Pyridyl-functionalized triarylamines self-assembled on Au(111) — •Leonid Solianyk[1], Juan Carlos Moreno-López[1], Jun Li[1], Stefano Gottardi[1], Ute Meinhardt[2], Milan Kivala[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [2]Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Germany

The formation of 2D molecular architectures on surfaces with both a predefined structure and desired catalytic/electronic properties is of potential interest for the usage in future nanoelectronic devices while self-assembly is a valuable tool for building these nanostructures. In our work, we investigated the self-assembly of pyridyl-functionalized triarylamines on the Au(111) surface by scanning tunneling microscopy at 77K and low energy electron diffraction. For deposition of submonolayer coverage onto Au(111) held at room temperature, a close-packed phase as well as a hexagonal nanoporous network were observed to coexist. The close-packed phase is stabilized by hydrogen bonding while the nanoporous network is held together by metal-ligand interactions with native gold atom(s). Thermal annealing at 180°C results in the exclusive formation a second hexagonal nanoporous network with a larger pore size. The structural models and the intermolecular as well as the molecule substrate interactions are discussed for the mentioned structures.

O 37.5 Tue 15:15 S054

Self-assembly and on-surface coupling of a carbonyl-bridged triphenylamine derivative — •Maximilian Ammon[1], Zechao Yang[1], Tim Sander[1], Patrick Seitz[1], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, FAU Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg, Germany

Carbonyl-bridged triphenylamines are versatile planar π-systems for the formation of self-assembled and covalent honeycomb networks. Here we present a low-temperature scanning tunneling microscopy (STM) study on the self-assembly of amino-functionalized carbonyl-bridged triphenylamine derivatives. On Au(111), we find hydrogen-bonded porous networks after evaporation at room temperature. The bonding motif is similar to the one expected in gas phase, which demonstrates a weak molecule-surface interaction. In contrast on Ag(111) the strong interaction between the carbonyl groups and the metal promotes metal-ligand bonded networks at room temperature. The bridging carbonyl groups are suitable for Schiff-base type coupling reactions, which proceed, compared to the Ullmann coupling, at lower temperatures and leave no reaction side products on the surface [1]. We will discuss results on the covalent coupling by post annealing on both surfaces.

[1] S. Weigelt, C. Busse, C. Bombis, et al., Angewandte Chemie 119, 9387-9390 (2007)

O 37.6 Tue 15:30 S054

On-Surface Reductive Coupling of Aldehydes on Au(111) — •Oscar Díaz Arado[1,2], Harry Mönig[1,2], Jörn-Holger Franke[3], Alexander Timmer[1,2], Philipp Held[4], Armido Studer[4], and Harald Fuchs[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Deutschland — [2]Center for Nanotechnology (CeNTech), Münster, Deutschland — [3]Department of Physics, Université Libre de Bruxelles, Bruxelles, Belgium — [4]Organisch-Chemisches Institut, Westfälische Wilhelms-Universität, Münster, Deutschland

The on-surface covalent coupling of organic molecules has been shown to have great potential as a promising approach for the bottom-up design of novel functional organic nanomaterials. Herein we report the C-C coupling of a terephthaldehyde to produce polyphenylene vinylene oligomers on a Au(111) surface. Scanning tunneling microscopy and photoelectron spectroscopy experiments revealed the success of the covalent coupling after oxygen dissociation and subsequent desorption from the surface. These results, together with density functional theory calculations, showed that the typical diolate-mediated reaction mechanism for the reductive coupling of carbonyls does not apply in this case. Instead, the reaction proceeds after C-H activation of the aldehyde moiety followed by a two-step deoxygenation process involving reactive sites on the substrate. With this on-surface synthesis approach, nanostructures with tunable optoelectronic properties on substrates can be developed, thus increasing the existing pool of suitable reactions for the growth of organic nanostructures on surfaces.

O 37.7 Tue 15:45 S054

Disaccharide self-assembly on metal surfaces — •Sabine Abb[1], Ludger Harnau[1], Christian Schön[1], Juan Cortés[2], Stephan Rauschenbach[1], and Klaus Kern[1,3] — [1]Max Planck Institute for solid state research, Stuttgart, Germany — [2]Centre national de la rechereche scientifique, LAAS, Toulouse France — [3]Ecole Polytechnique Fédérale de Lausanne, Switzerland

Saccharides are involved in almost every biological process, including signal transducing, cell-adhesion and differentiation. However, the interactions of saccharides adsorbed on a surface are not well understood on a molecular level. While the physical properties differ, the chemical structure of the monosaccharide building blocks is very similar - they all are structural and stereo isomers of the chemical sum formula $C_6H_{12}O_6$. Their vastly different behavior follows from rather subtle differences in the placement of OH-groups in the molecules.

In this study we investigate the self-assembly of the disaccharides sucrose and trehalose on Cu(100) by STM. Electrospray ion beam deposition (ES-IBD) enables us to deposit these non-volatile molecules on the surface in ultra-high vacuum as negatively charged molecular ions. After deposition of a submonolayer coverage, we observe self-assembly of ordered 2D nanostructures as well as single molecules.

Based on our observations combined with molecular dynamics and energy landscape calculations, we can propose a model for the different disaccharide assemblies elucidating the influence of the isomers on the assembly behavior. Moreover, imaging of saccharides may be applicable to characterize branched polysaccharides.

O 38: Spintronics

Time: Tuesday 14:00–16:00 Location: S051

O 38.1 Tue 14:00 S051

Skyrmion à la carte: Engineering magnetic skyrmions at transition-metal multilayers — •Bertrand Dupé[1], Gustav Bihlmayer[2], Marie Böttcher[1], Stefan Blügel[2], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel, 24098 Kiel, Germany — [2]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Due to their unique topological and dynamical properties skyrmions in magnetic materials offer attractive perspectives for future spintronic applications [1]. Recently, it has been discovered that magnetic skyrmions can also occur in ultra-thin transition metal films at surfaces [2,3]. However, so far only skyrmions at interfaces with a single atomic layer of a magnetic material were reported, which greatly limits their potential for application in devices. Here, we predict the emergence of skyrmions in $[4d/\mathrm{Fe}_2/5d]_n$ multilayers, i.e. structures composed of Fe biatomic layers sandwiched between 4*d*- and 5*d*-transition-metal layers [4]. In these composite structures, the exchange and the Dzyaloshinskii-Moriya interactions, which control skyrmion formation, can be tuned separately by the two interfaces. This allows engineering skyrmions as shown by density functional theory and spin dynamics simulations. [1] A. Fert, *et al.*, Nature Nano. **8**, 152 (2013). [2] N. Romming, *et al.*, Science **341**, 636 (2013). [3] B. Dupé, *et al.*, Nature Comm. **5**, 4030 (2014). [4] B. Dupé, *et al.*, submitted (arXiv :1503.08098).

O 38.2 Tue 14:15 S051

Multichannel-Spin-Polarimetry for the Analysis of Spin-Transport in Metal-Organic Interfaces — •Erik Schaefer[1,2], Martin Krämer[1], Dmytro Kutnyakhov[1], Katerina Medjanik[1], Gerd Schönhense[1,2], and Hans-Joachim Elmers[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz — [2]Graduate School Materials Science in Mainz, Mainz

Spin- and angular resolved photoemission spectroscopy has become the key technique for the investigation of electronic properties of promising spintronic materials. In contrast to conventional photon optics, an effective spin polarization analysis of a given electron beam is difficult. Since organic materials tend to degrade within a short period, a massive reduction of spin-resolved data acquisition time is crucial. The recent developed multichannel spin- and angle-resolved photoemission spectroscopy [1] solves this issue by enhancing the figure of merit by several orders of magnitudes. Ir(001) shows high potential for the use as a scattering target in multichannel spin analysis [2]. A new Ir(001) multichannel spin-detection system was constructed and the important quantities and efficiency of the system were determined. Spin- and angle-resolved photoemission spectroscopy of thin iron films on W(110) were performed.

Founded by Stiftung Rheinland Pfalz für Innovation (project 1038)
[1] M. Kolbe et al., Phys. Rev. Lett. 107, 207601 (2011)
[2] D. Kutnyakhov et al., Ultramicroscopy 130, 63-69 (2013)

O 38.3 Tue 14:30 S051

Spin-resolved ToF momentum-microscopy of anomalous surface states on W(110) — •D. Kutnyakhov[1], S.V. Chernov[1], R. Wallauer[1], K. Medjanik[2], S.A. Nepijko[1], C. Tusche[3], M. Ellguth[3], S. Borek[4], J. Braun[4], J. Minár[4,5], H. Ebert[4], H.J. Elmers[1], and G. Schönhense[1] — [1]Institut für Physik, Uni-Mainz — [2]MAX IV Lab., Lund, Sweden — [3]MPI für Mikrostrukturphysik, Halle — [4]Dep. Chemie, LMU München — [5]University of West Bohemia, Pilsen, Czech Republic

Spin-resolved bandmapping of anomalous surface states on W(110) has been performed via time-of-flight (ToF) momentum microscopy with an imaging spin-filter using synchrotron radiation at the beamline U125-NIM at BESSY II (hν=22 eV). 3D (k_x,k_y,E_B)-maps in the full surface Brillouin zone with 3.4 Å^{-1} dia. and 4 eV binding energy range were measured simultaneously, resolving 2.5×10^5 voxels without and more than 10^4 voxels with spin resolution. Similar to our recent experiment on Mo(110) [1] the results give evidence for d-like surface resonances in the spin-orbit induced partial band gap. In agreement with previous results [2], we find the dispersing state with Dirac-like signature and Rashba spin texture crossing the bandgap at the $\overline{\Gamma}$-point and E_B=1.25 eV. A second linear band crossing occurs close to the midpoint between $\overline{\Gamma}$ and $\overline{\mathrm{N}}$ at E_B=0.8 eV. Results are compared with one-step photoemission calculations in its density matrix formulation.

Funded by BMBF (05K13UM1, 05K12EF1, 05K13WMA). [1] Chernov et al., Ultramicroscopy, (2015), doi:10.1016/j.ultramic.2015.07.008; [2] Miyamoto et al., PRL 108, 066808 (2012)

O 38.4 Tue 14:45 S051

Spin-polarized electron energy loss spectrometer with detection of final state spin polarization — •Dmitry Vasilyev and Jürgen Kirschner — Max-Planck Institut für Mikrostrukturphysik, Halle, Germany

Spin polarized electron energy loss spectroscopy (SPEELS) allows to investigate Stoner excitations, as was demonstrated 30 years ago. Based on theory one should expect structured energy loss spectra with features on the scale of less than 1 eV. The spectra should change with varying the incidence angle by a few degrees, and the primary energy of electrons by less than 1 eV. However, this was not observed at that time. We have developed a new SPEELS apparatus with the detection of final state spin polarization. The new spectrometer allows us to see all the expected features. Spin-polarized electrons are generated via photoemission from GaAs-based superlattice. The direction of the electron spin can be changed by varying the light helicity. Additionally the magnetization of the target can be reversed. A multichannel spin detector is used for the measurement of the spin-polarization of the outgoing electrons. It is based on spin dependent reflection from pseudomorphic Au on Ir (001). This system provides high polarization sensitivity, up to 80%, and more that 8 months lifetime in ultrahigh vacuum. The measurement of intensity asymmetries for opposite magnetization directions allows to distinguish between spin-orbit asymmetry and exchange asymmetry. Together with detection of the spin-polarization of the outgoing electrons it allows to determine relative transition probabilities for each of the four partial intensities.

O 38.5 Tue 15:00 S051

Ab initio investigation of a novel spin-filter: Graphene on Ir(111) — •Christian Mende[1], Stephan Borek[1], Jürgen Braun[1], Gustav Bihlmayer[2], Dima Kutnyakhov[3], Hans-Joachim Elmers[3], Gerd Schönhense[3], Jan Minár[1,4], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universität München — [2]Forschungszentrum Jülich — [3]Johannes-Gutenberg-Universität Mainz — [4]University of West Bohemia Pilsen

For the determination of the spin-polarized band structure in angle-resolved photoemission (ARPES) experiments an application of materials as reflection mirrors is recommended. For this purpose one uses the spin-dependent scattering of photoelectrons from suitable surfaces based on either exchange or spin-orbit induced scattering. We present our calculations of spin-polarized low energy electron diffraction (SPLEED) patterns for the clean Ir(111) and the Graphene covered Ir(111) surface. For these materials the electron scattering is strongly influenced by spin-orbit interaction whereas the Graphene layer provides a longer lifetime of the spin-polarizing mirror due to its inert properties concerning surface contamination. Based on ab initio calculations of the electronic structure we obtained diffraction patterns over a wide range of kinetic energies and polar angles to determine the applicability of the Ir(111)+Graphene system as spin-polarizing mirror. Additionally we investigated ARPES spectra to connect the electronic structure calculations to the corresponding experiment.

O 38.6 Tue 15:15 S051

Ab initio calculation of SPLEED patterns for the Ir(111) surface — •Stephan Borek[1], Jürgen Braun[1], Jan Minár[1,2], Dima Kutnyakhov[3], Hans-Joachim Elmers[3], Gerd Schönhense[3], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universität München — [2]University of West Bohemia Pilsen — [3]Johannes-Gutenberg-Universität Mainz

Recent investigations have shown that the Ir(100) surface is a promising candidate for spin-filter application [1]. In our studies we investigated the Ir(111) surface and its applicability for spin-filter purposes. Accordingly, diffraction patterns of spin-polarized electrons scattered on the surface have been calculated for a wide range of polar angles and kinetic energies. The calculated diffraction patterns show more suitable working points in comparison to the standard Ir(100) surface extending the spin-filter versatility. In addition we looked for deviations of the scattering plane from high symmetry directions $\overline{\Gamma}\,\overline{M}$ and $\overline{\Gamma}\,\overline{K}$ in the surface Brillouin zone and its impact on the diffraction patterns. To complement the SPLEED calculations we calculated angle-resolved photoemission spectra to characterize the underlying electronic structure.
[1] D. Kutnyakhov et al. Ultramicroscopy **130**, 63 (2013)

O 38.7 Tue 15:30 S051

Determining excitation pathways at the Cobalt/Alq3 interface — •Philip Thielen[1,2], Anna-Katharina Mahro[1], Benjamin Stadtmüller[1], Mirko Cinchetti[1], and Martin Aeschlimann[1] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Gottlieb-Daimler-Str. 47, 67663 Kaiserslautern, Germany

One of the fundamental questions in molecular spintronics consists in understanding the properties of hybrid interfaces between molecules and ferromagnetic metals. Recently, it was shown that the interface state between a thin layer of the metalorganic complex tris(8-hydroxyquinolinato)aluminium (Alq3) and a cobalt surface acts as a spin filter due to the prolonged spin-dependent trapping of electrons [1]. The excitation of spin-polarized electrons into such hybrid interface states can take place either directly from the cobalt in a coherent process or in an indirect, incoherent process, e.g. via charge transfer. We show that we can disentangle coherent and incoherent excitation pathways using a phase-stabilized two-pulse correlation experiment. We discuss the possible implications of our findings regarding the optical control of spin-polarized electrons at hybrid interfaces.

References: [1] S. Steil, N. Großmann, M. Laux, A. Ruffing, D. Steil, M. Wiesenmayer, S. Mathias, O. L. A. Monti, M. Cinchetti and M. Aeschlimann, Nature Physics 9, 242 - 274 (2013)

O 38.8 Tue 15:45 S051

Energy Dispersion and Spin Structure of Unoccupied States of BiTeI: A Matter of Surface Termination? — •Christian Langenkämper[1], Koji Miyamoto[1], Anke B. Schmidt[1], Peter Krüger[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany

We present a combined experimental and theoretical study on the unoccupied electronic structure of BiTeI along the $\overline{\Gamma}$-$\overline{\mathrm{K}}$ direction. We performed spin-resolved inverse-photoemission experiments on samples with different surface termination, Te and I.

For the two surface terminations we found distinct differences in the energy dispersion of the surface states around $\overline{\Gamma}$, which are caused by band bending. In contrast, this effect is not observed around the $\overline{\mathrm{K}}$ point. With the help of *ab initio* band-structure calculations we identify the observed states as bulk states, not influenced by band bending.

In addition, we studied the spin structure of the unoccupied bands. Around the $\overline{\Gamma}$ point, we found a Rashba-type in-plane spin polarization. Upon approaching $\overline{\mathrm{K}}$, the direction of the spin polarization rotates from fully in-plane to out-of-plane. This spin texture is in accordance with the crystal symmetry and independent of the surface termination.

O 39: 1D Metal Wires on Semiconductors II

Time: Tuesday 14:00–16:00 Location: S052

O 39.1 Tue 14:00 S052

Infrared Plasmonic Investigation of Band Filling-Induced Metal-to-Insulator Transition in Au Chains on Si(111)-5x2-Au — •Fabian Hötzel[1], Kaori Seino[2], Friedhelm Bechstedt[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Deutschland — [2]Institut für Festkörpertheorie und -optik, Universität Jena, Jena, Deutschland

The investigation of infrared plasmon polaritons on the Si(111)-5x2-Au surface underlines the metallic character of the system [1] and its Kwon-Kang atomic structure model [2] with seven Au atoms per 5x2 surface unit cell. However, upon evaporating an additional 0.1 monolayer Au amount, the system undergoes a metal-to-insulator transition [3] but the 5x2 symmetry remains unchanged as proven by reflection high energy electron diffraction. This phase transition was in situ observed by means of the infrared plasmonic signal attenuation with coverage. Band-structure calculations reveal that the transition is induced by band filling of the one-dimensional half-filled band at the Fermi energy. The insulating phase represents an indirect semiconductor with a band gap of 0.29 eV. Moreover, a new surface structure model with eight Au atoms per unit cell, including the additional Au atoms, is developed for the 5x2 symmetry. By annealing the system, the plasmonic signal is recovered which shows that the phase transition is reversible. This contribution is part of the DFG Research Unit FOR 1700.
[1] Hötzel, F. et al. Nano Lett. **2015**, 15, 4155-4160.
[2] Kwon, S. G. et al. Phys. Rev. Lett. **2014**, 113, 086101.
[3] Hötzel, F. et al. J. Phys. Chem. Lett. **2015**, 6, 3615-3620.

O 39.2 Tue 14:15 S052

Optical monitoring of Ag nanostructures on Si(557) — •Sandhya Chandola[1], Eugen Speiser[1], Jochen Räthel[1], Ulrich Krieg[2], Christoph Tegenkamp[2], Herbert Pfnür[2], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany — [2]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167, Hannover, Germany

The optical response of the Si(557)-Ag surface has been studied with reflectance anisotropy spectroscopy (RAS) from 0.5 to 5 eV. Using the Si(557) surface as a template, various quasi-one dimensional (1D) Ag structures were grown and substantial differences between the structures were observed with RAS. At $\sim$ 0.3 ML of Ag, 1D chain structures were observed with STM and a large anisotropic response developed at 2.5 eV, related to the formation of Ag nanowires which are semiconducting. Further deposition up to 1.2 ML of Ag resulted in the formation of the $(\sqrt{3}\times\sqrt{3})$ phase. The anisotropy at 2.5 eV disappeared and the overall optical response showed substantial modification. Small amounts of Ag, from 0.03 ML to 0.1 ML of Ag, were then deposited on the $(\sqrt{3}\times\sqrt{3})$ surface to monitor the effects of doping on these structures. The RAS response showed a significant anisotropy towards the infrared for small amounts of doping. As RAS is only sensitive to the anisotropic optical response, which arises from stepped and facetted regions of the surface, it can be a sensitive tool to monitor the effects of excess Ag atoms concentrated at the step sites of the Si(557) surface which are supposed to be responsible for the doping mechanism.

O 39.3 Tue 14:30 S052

Fabrication of one-dimensional arrays of magic clusters using a vicinal Si surface as a template — •Martin Franz, Julia Schmermbeck, and Mario Dähne — Technische Universität Berlin, Institut für Festkörperphysik, 10623 Berlin, Germany

Self-assembled magic clusters on surfaces are fascinating not only from a fundamental scientific point of view, they are also promising candidates to employ such zero-dimensional nano objects in future applications such as high-density memory devices or in catalysis. In the present work, magic In clusters that form on the Si(111)7×7 surface are used as a model system to study how the array formation affects the electronic properties and to explore the possibility to produce one-dimensional (1D) arrays of magic clusters. For this purpose, scanning tunneling microscopy and spectroscopy are empoyed. The basic properties of these clusters, such as the atomic structure and the preparation procedure, are well known. In addition, it is possible to produce perfectly ordered two-dimensional (2D) arrays of these clusters on planar Si(111)7 × 7 samples. In the present work, different electronic properties and in particular different energy gaps are observed for clusters forming in the faulted and unfaulted half unit cell of the 7 × 7 reconstruction as well as for clusters neighboring other clusters. Furthermore, the Si(557) surface, which is a vicinal surface with narrow Si(111) terraces, is used as a template resulting in the formation of two different types of 1D arrays, similar to the two types of 2D arrays that are found on the planar Si(111) surface. This work was supported by the DFG through FOR 1282 project D.

O 39.4 Tue 14:45 S052

Selective One-Dimensional Growth of an Alkyl-Sugar Functionalized Ferrocene of Graphite — •Thiruvancheril Gopakumar, Prithwidip Saha, Khushboo Yadav, Shibin Chako, and Ramesh Ramapanicker — Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India

Ferrocene molecules are interesting class of semi-conducting organometallic molecules because of their excellent redox efficiency. In addition the redox potentials may be manipulated substantially by altering functional groups attached directly to Ferrocene. Here we show, using AFM, selective one-dimensional growth of an alkyl-sugar functionalized Ferrocene molecule on graphite basal plane. The assembly is driven by formation of Ferrocene dimers. The one-dimensional growth selectivity is further enhanced by adding a keto (-C=O) group in the alkyl part of alkyl-sugar group. The growth of elongated molecular islands is only limited by terrace edges or other molecular islands and is controlled by additional inter-dimer hydrogen bonding between keto group and alkyl -C-H groups.

O 39.5 Tue 15:00 S052

Growth and electronic structure of Tb disilicide nanowires on vicinal Si(111) surfaces — •Stephan Appelfeller, Martin Franz, Christian Hassenstein, Lars Freter, Hans-Ferdinand Jirschik, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

One-dimensional metals may be useful for future applications, but they are especially interesting due to their unique physical phenomena, e.g. Luttinger liquid behavior or the Peierls transition. Vicinal substrates can enable the formation of such nanowires, when thin metallic films grow exclusively on well separated, narrow terraces. $TbSi_2$ forms well ordered metallic monolayer films on planar Si(111) [1]. Here, the nanowire formation of $TbSi_2$ on various vicinal Si(111) samples was investigated. Structural information, e.g. dimensions and edge characteristics, were obtained by scanning tunneling microscopy and confirm, together with the electronic properties obtained by core-level photoemission spectroscopy, the growth of $TbSi_2$. Furthermore, the electronic dimensionality of the nanowires, which is illustrated by their Fermi surfaces, was determined using angle resolved photoemission spectroscopy.

This work was supported by the DFG (FOR1700, project E2). We kindly acknowledge the support of K. Horn and coworkers and of BESSY, where the photoemission experiments were carried out at the beamlines UE56/2 PGM-1 and PGM-2.

[1] M. Franz, J. Große, R. Kohlhaas, and M. Dähne, Surface Science **637**, 149 (2015).

O 39.6 Tue 15:15 S052

Strain induced quasi one-dimensional rare earth silicides structures on Si(111) — •Frederic Timmer[1], Robert Oelke[1], Martin Franz[2], Stephan Appelfeller[2], Mario Dähne[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Rare earth elements (REE) covered silicon surfaces have been in the focus of research for more than 30 years due to their unique properties. For instance, thin REE-silicide films on n-type Si(111) possess very low Schottky-barriers in conjunction with an abrupt surface making them interesting as ohmic contacts. Furthermore REE-nanowires might be applicable as interconnects in future nanodevices or as plasmonic waveguides due to their quasi one-dimensional structure.

Here, we report on a $\left(2\sqrt{3} \times \sqrt{3}\right)$ R30° reconstruction for REE coverages exceeding 1 ML which is therefore related to the well-known $\left(\sqrt{3} \times \sqrt{3}\right)$ R30° reconstruction. We characterize the structure of the silicide films by means of Low Energy Electron Diffraction (LEED) including Spot Profile Analysis (SPA-LEED) and Scanning Tunneling Microscopy (STM). The stoichiometry of the films and their growth mode is studied by Auger Electron Spectroscopy (AES). Combining experimental results, we develop a complex model for the reconstructed surface including formation of quasi one-dimensional structures, due to striped domains.

O 39.7 Tue 15:30 S052

Local transport measurements on terbium-silicide nanowires — •Frederik Edler[1], Ilio Miccoli[1], Herbert Pfnür[1], Stephan Appelfeller[2], Mario Dähne[2], Simone Sanna[3], Wolf G. Schmidt[3], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover — [2]Institut für Festkörperphysik, TU Berlin, 10623 Berlin — [3]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33098 Paderborn

Metal silicide wires play an important role in electronics as ohmic contacts and gate electrodes due to their very low resistivity. Rare-earth (RE) metals (eg. Tb, Dy, Er, Y) can be used to grow long, extremely thin nanowires because of uniaxial lattice matching with Si which could be used for additional downscaling of Si based technology.

The transport properties of Tb silicide wires have been studied via 4-tip STM/SEM system. The SEM allows a fast characterization of sample quality and precise positioning of feedback controlled STM tips, enabling gentle contacts and transport measurements on a nm-scale. Moreover, the STM was used to correlate the surface morphology of nanowires with transport findings.

Our measurements reveal three types of metallic wires mainly depending on the growth parameters. Further analysis shows that the resistivity is strongly depending on the height of wires, which is increased for small heights. The data can be perfectly described by a theoretical model taking into account the surface roughness and lateral surface correlation. STS reveals that the wires are electronically decoupled from the Si substrate in agreement with recent DFT calculations.

O 39.8 Tue 15:45 S052

Capping of rare earth silicide nanowires on Si(001) — •Stephan Appelfeller[1], Martin Franz[1], Milan Kubicki[1], Paul Reiss[2], Tore Niermann[2], Markus Andreas Schubert[3], Michael Lehmann[2], and Mario Dähne[1] — [1]Institut für Festkörperphysik, TU Berlin, 10623 Berlin — [2]Institut für Optik und Atomare Physik, TU Berlin, 10623 Berlin — [3]IHP - Leibniz-Institut für innovative Mikroelektronik, 15236 Frankfurt (Oder)

Rare earth silicide nanowires are promising candidates for the use of one-dimensional metals in future applications, but they are not stable under ambient conditions. Thus, a protective layer is needed. Here, the capping of Tb and Dy silicide nanowires grown on Si(001) by Si overlayers was studied using scanning tunneling microscopy and cross-sectional high-resolution transmission electron microscopy, also with energy dispersive X-ray analysis. Amorphous Si films deposited at room temperature allow an even capping, while the nanowires maintain their original structural properties. Subsequent recrystallization by thermal annealing leads to more compact nanowire structures and to troughs in the Si layer above the nanowires, which may even reach down to the nanowires in the case of thin Si films, as well as to V-shaped stacking faults forming along {111} lattice planes. This behavior is most probably related to strain due to the lattice mismatch between the Si overlayer and the nanowires.

This work was supported by the DFG (FOR1700, project E2).

O 40: Heterogeneous Catalysis: Experiment

Time: Tuesday 14:00–16:00 Location: S053

O 40.1 Tue 14:00 S053

Bimetallic redox interactions in model Pt-Sn-CeO$_2$ catalysts for fuel cell applications — •A. Neitzel[1], Y. Lykhach[1], N. Tsud[2], T. Skála[2], M. Vorokhta[2], K. C. Prince[3], V. Matolín[2], and J. Libuda[1] — [1]FAU Erlangen-Nürnberg, Germany — [2]Charles University in Prague, Czech Republic — [3]Elettra-Sincrotrone Trieste, Italy

We investigated bimetallic Pt-Sn interactions as a function of the oxidation state of Pt and Sn in model Pt-Sn-CeO$_2$ catalysts by synchrotron radiation photoelectron spectroscopy and resonant photoemission spectroscopy. The corresponding experiments involved model Sn-CeO$_2$ and Pt-CeO$_2$ mixed oxide films prepared on a stoichiometric CeO$_2$(111) buffer layer on Cu(111). Both systems are characterized by excellent stabilities of Sn^{2+} and Pt^{2+} upon annealing to 700 K in UHV. We found that deposition of metallic Sn^0 on Pt-CeO$_2$ films initially leads to formation of Pt-Sn-CeO$_2$ mixed oxides. At larger amounts of Sn^0, we observed conversion of Pt^{2+} to new species which we assign to small Pt or PtO$_x$ particles. The following annealing of the deposit to 700 K in UHV leads to complete reduction of Pt^{2+} but does not yield Pt-Sn alloy nanoparticles. Stepwise deposition of Pt on Sn-CeO$_2$ films yields Pt-Sn alloy nanoparticles at the expense of Sn^{2+}. Subsequent annealing of the deposit in UHV to 750 K promotes further Pt-Sn alloy formation. The surface composition of Pt-Sn-CeO$_2$ catalysts was probed by CO adsorption at 110 K. We found that CO adsorption at atop sites on the Pt-Sn nanoparticles is inhibited due to thermally promoted alloying.

O 40.2 Tue 14:15 S053

Physical and chemical properties of Au nanoparticles on CeO$_2$ supports in the CO oxidation reaction — •Joachim Bansmann[1], Gabriela Kucerova[1], Ayman Abd El-Moemen[2], Ali Abdel-Mageed[1], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Chemistry Department, Suez Canal University, Ismailia, Egypt

Au nanoparticles (NPs) on metal oxide surfaces are interesting catalysts in the CO oxidation and water-gas shift (WGS) reaction. Here, we will focus on the influence of different oxidic and reductive pretreatments of Au/CeO$_2$ catalysts on the size and the oxidation state of the Au NPs using ex-situ characterization techniques (XRD and XPS) as well as in-situ methods such as XANES/EXAFS and diffuse IR spectroscopy (DRIFTS). Reductive pre-treatments in CO generally lead to smaller metallic particles, whereas the presence of oxidic species results in slightly larger and partially oxidic Au NPs.

Moreover, using these in-situ spectroscopy techniques, we followed the changes in the Au particle size and chemical state in the CO oxidation reaction after the different pre-treatments. Sintering/Ostwald ripening process affect the catalytic activity by lowering the surface area of Au which contributes to a decreasing reactivity. Additionally, DRIFTS measurements offer insight into adsorption sites of CO on Au NPs and the formation of carbonates and formates, which often block active site in the CO oxidation reaction.

O 40.3 Tue 14:30 S053

Surface oxide on Pt(111) as the active phase for NO and CO oxidation — •Matthijs van Spronsen[1], Joost Frenken[1], and Irene Groot[2] — [1]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands — [2]Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands

Pt find its main application in the automotive industry as a catalytic converter. As catalyst, Pt transforms harmful exhaust gases to more environment-friendly components. Technical catalysts are complex and is often obscuring fundamental processes. Therefore, model catalysts are frequently used. The simplest model catalyst is the close-packed (111) surface. Even though this model catalyst has been studied for over 45 years, the main questions remain unsolved. How does Pt oxidize? What is the atomic structures of the oxide(s)? And are the structures stable under chemical reaction conditions?

We studied the oxidation of Pt(111) with the ReactorSTM, which is an STM integrated with a small flow reactor. It allows to study the atomic structure of surfaces under chemical reaction conditions (high p & T).

This resulted in the observation of two novel structures, which were identified as single-layer thick surface oxides. The first one consisted of triangles forming spoked wheels, while the second one was a lifted-row oxide. Both structures were also observed under NO oxidation reaction conditions. These oxides contain weakly-bound oxygen atoms, which should be very reactive.

O 40.4 Tue 14:45 S053

CO and D$_2$O chemistry on continuous and discontinuous samaria thin films on Pt(111) — Jin-Hao Jhang[1], •Simona Keil[1], Andreas Schaefer[2], Volkmar Zielasek[1], and Marcus Bäumer[1] — [1]Institute of Applied and Physial Chemistry, University of Bremen, Germany — [2]Division of Synchrotron Radiation Research, Lund University, Sweden

The water-gas shift (WGS) reaction is among the most relevant for sustainable chemistry and energy conversion. Exemplarily for mixed metal – rare earth oxide WGS catalysts, the chemistry of CO and D$_2$O, individually adsorbed or co-adsorbed, on epitaxial thin films and islands of samaria on Pt(111) was studied by temperature programmed desorption spectroscopy in ultra-high vacuum. The comparative study indicates that Sm$_2$O$_3$ islands provide lattice oxygen at their perimeter for oxidation of CO adsorbed on adjacent Pt area. However, the reduced SmO$_x$ islands are not fully reoxidized by subsequent exposure to D$_2$O. Upon CO and D$_2$O coadsorption, interaction between CO and OD species at the perimeter of SmO$_x$ islands promotes D$_2$ formation but does not yield CO$_2$ as product. The study demonstrates the relevance of structural details at interface sites between metal and oxide for chemical reactions.

O 40.5 Tue 15:00 S053

High-pressure scanning tunneling microscopy during hydrodesulfurization catalysis — •Rik V. Mom[1], Joost W.M. Frenken[1,2], and Irene M.N. Groot[3] — [1]Huygens-Kamerlingh Onnes Laboratory, Niels Bohrweg 2, Leiden, The Netherlands — [2]Advanced Research Center for Nanolithography, Science Park 104, Amsterdam, The Netherlands — [3]Gorlaeus Laboratories, Einsteinweg 55, Leiden, The Netherlands

Many catalysts show reversible physical and chemical changes during operation. To capture these changes, *in situ* studies at elevated temperatures and pressures are essential. Using a home-built high-pressure scanning tunneling microscope we have studied reversible changes during the desulfurization reaction, in which sulfur is removed from hydrocarbons.

$C_xH_yS + H_2 \rightarrow C_xH_y + H_2S$

To mimic the industrial catalyst, MoS$_2$ nanoparticles were deposited on Au(111). We have studied the surface dynamics of this model catalyst during the conversion of CH$_3$SH to CH$_4$ in 1 bar of various CH$_3$SH/H$_2$ mixtures at temperatures up to 250°C. From our observations, it is clear that the atomic arrangement of the active sites depends on the gas environment. We show that the sulfur coverage of the active sites during catalysis is higher than expected from DFT equilibrium calculations [1]. We show that this can be explained by kinetic effects based on the high-energy barriers involved in the reaction.

[1] Lauritsen et al., Journal of Catalysis 221 (2004) 510-522

O 40.6 Tue 15:15 S053

In situ probing of structural changes in hydrogen activation over ceria/Ru inverse model catalysts — •Jan Ingo Flege[1], Jan Höcker[1], T. Onur Mentes[2], Alessandro Sala[2], Andrea Locatelli[2], Thomas Schmidt[1], Sanjaya D. Senanayake[3], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, Bremen, Germany — [2]Sincrotrone Elettra, Trieste, Italy — [3]Chemistry Department, Brookhaven National Lab, United States

Ceria is a highly versatile oxide and used in many catalytic applications today; however, its structure-function relation and true active nature in chemical redox reactions are still not well understood. An important example is the interaction of ceria with molecular hydrogen, which is an integral part of the hydrogenation process that produces methanol from CO$_2$. Here, employing a powerful combination of electron spectromicroscopy with synchrotron radiation, low-energy electron microscopy (LEEM), and micro-illumination diffraction analysis, we follow *in situ* the complex structural transformations of a well-defined ceria/Ru(0001) model catalyst system when exposed to a reactive H_2 environment [1]. We demonstrate that the transition from CeO_2 to crystalline Ce_2O_3 occurs through a mixture of transient, ordered cerium oxide phases whose average size is on the order of just a few nanometers. Furthermore, these crystalline surface phases are shown to exhibit characteristic intensity-voltage curves in low-energy electron microscopy, which allow their spatial distribution to be imaged in real space directly.

[1] J. Höcker *et al.*, Adv. Mater. Interfaces, in press (2015).

O 40.7 Tue 15:30 S053

Yet another view on catalysts: probing surface roughness with nm-scale sensitivity using visible light — •Andriy Taranovskyy[1], Willem Onderwaater[1,5], Gertjan van Baarle[1,2], Irene Groot[3], and Joost Frenken[4] — [1]Leiden Institute of Physics, Leiden, The Netherlands — [2]Leiden Probe Microscopy BV, Leiden, The Netherlands — [3]Leiden Institute of Chemistry, Leiden, The Netherlands — [4]ARCNL, Amsterdam, The Netherlands — [5]ESRF, Grenoble, France

We have developed a flow reactor with an optical window which allows us to measure the reflectivity of a catalytically active sample using a 625nm light source. We will show that we can relate the reflectivity to surface roughness, even if the correlation length of the roughness is much smaller than the wavelength of the light. We will show that using this technique we can follow the roughening/smoothening of a Pd(100) surface in space and time during switches between the oxidized and metallic state. We conclude that this easy yet powerful technique provides complementary information to more local probes such as STM and SXRD.

O 40.8 Tue 15:45 S053

***In-situ* temperature measurement using chemoelectronic nanodiodes** — •Jan Philipp Meyburg, Detlef Diesing, and Eckart Hasselbrink — Fakultät für Chemie, Universität Duisburg-Essen, Essen, Germany

Chemoelectronic nanodiodes based on metal–insulator–metal thin film structures allow the detection of hot charge carriers that are excited in the course of surface reactions. In this context, the Pt-catalyzed oxidation of carbon monoxide is studied on a Pt–Ta_2O_3–Ta nanodiode. In order to activate this surface reaction locally the nanodiode is heated while the sample holder is held at a constant temperature below 80 K. Thus, a temperature gradient results and an accurate *in-situ* temperature measurement is required. During a continuous variation of the potential between the Pt electrode and the Ta electrode a device current is recorded that exhibits a temperature dependence. Consequently, this current can be used in order to monitor the device temperature. Therewith, exclusively the temperature of the nanoscopic MIM volume is measurable during the reaction process.

O 41: Frontiers of Electronic Structure Theory: Focus on Topology and Transport I

Time: Tuesday 14:00–16:00 Location: H24

Topical Talk O 41.1 Tue 14:00 H24

Topological semimetals and chiral transport in inversion asymmetric systems — •Shuichi Murakami — Department of Physics and TIES, Tokyo Institute of Technology, Tokyo, Japan

Weyl semimetals (WS) are semimetals with nondegenerate 3D Dirac cones in the bulk. We showed that in a transition between different Z2 topological phases, the Weyl semimetal phase necessarily appears when inversion symmetry is broken. In the presentation we show that this scenario holds for materials with any space groups without inversion symmetry. Namely, if the gap of an inversion-asymmetric system is closed by a change of an external parameter, the system runs either into (i) a Weyl semimetal phase or (ii) a nodal-line semimetal, but no insulator-to-insulator transition happens. This transition is realized for example in tellurium (Te). Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation. We also theoretically propose chiral transport in systems with such helical structures.

O 41.2 Tue 14:30 H24

Topological orbital magnetic moments — •Manuel dos Santos Dias, Juba Bouaziz, Mohammed Bouhassoune, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Orbital magnetic moments are usually associated with the spin-orbit interaction (SOI). We explore from first-principles how topological orbital magnetic moments (TOMs) can emerge in non-trivial magnetic spin textures, even without SOI, justifying the ‘topological’ label. Firstly, the case of magnetic trimers on the Cu(111) surface illustrates the basic symmetry properties of the TOMs, and how to separate their contribution from the usual SOI-driven orbital moments. We then focus on the implications of TOMs for single magnetic skyrmions formed in Pd/Fe/Ir(111) [1], considering their possible use in detecting and distinguishing skyrmions from anti-skyrmions by optical means.

Work funded by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] D.M. Crum et al., Nat. Comms. **6**, 8541 (2015)

O 41.3 Tue 14:45 H24

The orbital Rashba effect — •Dongwook Go[1,2], Patrick Buhl[1], Gustav Bihlmayer[1], Yuriy Mokrousov[1], Hyun-Woo Lee[2], and Stefan Blügel[1] — [1]Institute for Advanced Simulation and Peter Grünberg Institut, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics, Pohang University of Science and Technology, 37673 Pohang, Korea

We present a new surface phenomenon called the *orbital* Rashba effect, analogous to the spin Rashba effect. The effect is described by the orbital Rashba Hamiltonian, $H_{\mathrm{orb\text{-}R}}(\mathbf{k}) = \alpha_{\mathrm{orb\text{-}R}}\mathbf{L}\cdot(\hat{\mathbf{z}}\times\mathbf{k})$, where $\mathbf{L}$ is the orbital moment derived from atomic orbitals and $\alpha_{\mathrm{orb\text{-}R}}$ is the orbital Rashba constant. This leads to orbital-dependent energy splittings and orbital texture in the $\mathbf{k}$-space. The mechanism behind the emergence of the $H_{\mathrm{orb\text{-}R}}(\mathbf{k})$ can be understood as the $\mathbf{k}$-dependent magnetoelectric coupling due to atomic orbital hybridization. In the presence of intra-atomic spin-orbit coupling, the spin moment is aligned parallel or antiparallel to the orbital moment, thus the spin Rashba effect is recovered. As an example, we present a tight-binding and an *ab initio* study of the Bi/Ag(111) surface alloy, where the hybridization between a Ag *s*-orbital and a Bi *p*-orbital leads to the orbital Rasbha effect that is dominant over the spin one. The orbital Rashba effect is a key to new physics and to understanding spin-orbit driven physics at surfaces and interfaces, such as Dzyaloshinskii-Moriya interaction, non-collinear magnetism, etc.

O 41.4 Tue 15:00 H24

Spin and orbital magnetism of Rashba electrons induced by magnetic nanostructures — •Juba Bouaziz, Manuel dos Santos Dias, Phivos Mavropoulos, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We explore theoretically the spin and orbital magnetism of Rashba electrons in the presence of noncollinear impurity-induced magnetic states. The Rashba electron gas mediates the Dzyaloshinksii-Moriya interaction between magnetic impurities favoring chiral states [1]. Here we investigate the back-action of such noncollinear magnetic states on the Rashba electron gas. The presence and distribution of ground state spin and orbital currents is analyzed. Surprisingly, when switching off the spin-orbit coupling, chiral magnetic textures generate bound currents, which implies the existence of orbital magnetic moments originating solely from the peculiar topology of the impurities magnetic moments. In the particular case of a single adatom with an out of plane magnetic moment, we found circular currents flowing around the magnetic impurity in agreement with the continuity equation for the electric charge. Similar results were predicted for magnetic adatoms on superconductor surfaces with a finite spin-orbit coupling [2].

[1] J. Bouaziz *et al.* in preparation.
[2] S. S. Pershoguba *et al.* Phys. Rev. Lett. **115**, 116602 (2015).

This work is supported by the HGF-YIG Programme VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory).

O 41.5 Tue 15:15 H24

First-principles investigation of the impact of single atomic defects on magnetic skyrmions — •Imara L. Fernandes, Benedikt Schweflinghaus, Juba Bouaziz, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Chiral magnetic skyrmions are topological spin-swirling textures with rich physics and technological potential in the field of information storage. In a device, skyrmions certainly interact with defects and imperfections resulting into pinning phenomena. We explore from first-principles the non-trivial impact of 3d and 4d impurities on the energetics, electronic and magnetic properties of single magnetic skyrmions. Utilizing the newly developed Jülich full-potential relativistic Korringa-Kohn-Rostoker Green function method [1], we focus on topological magnetic objects of sub-5nm diameters stabilized in a single ferromagnetic layer of Fe sandwiched between the Ir(111) surface and one or two Pd layers, where the tunneling spin-mixing magnetoresistance (TXMR) was demonstrated theoretically [2] and experimentally [3]. – Funding provided by the HGF-YIG Program VH-NG-717 and the CNPq (BRAZIL).
[1] D. S. G. Bauer, Schriften des Forschungszentrum, Key Tech. **79** (2014).
[2] D.M. Crum *et al.*, Nat. Comms. **6**, 8541 (2015).
[3] C. Hanneken *et al.*, Nat. Nanotech. Doi:10.1038/nano.2015.218 (2015).

O 41.6 Tue 15:30 H24

Topological magnons: Any chance to find them? — •Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Topological magnon insulators (TMIs) have a nontrivial topology due to the Dzyaloshinskii-Moriya interaction which results in spatially confined edge states and, thus, energy and spin currents along their edges [1,2]. Several systems have been identified as TMIs, for example, Cu(1,3-benzenedicarboxylate) consisting of kagome planes [3], or the family of ferromagnetic pyrochlore oxides, e. g., $Lu_2V_2O_7$, showing the magnon Hall effect [4]. However, to date, no direct experimental evidence of a topological magnon band has been provided, what comes down to the small total width of the magnon dispersion relation and the energy resolution of surface sensitive measurements.

We propose Fe_3Sn_2 as promising candidate for a TMI. The total width of its magnon dispersion relation is large, and we determine its nontrivial topology by constructing an effective spin Hamiltonian. On this basis, we discuss signatures of topological magnon states that should be looked for in experiments.

[1] L. Zhang et al., PRB **87**, 144101 (2013); [2] A. Mook et al., Phys. Rev. B **89**, 134409 (2014); *eidem*, Phys. Rev. B **90**, 024412 (2014); *eidem*, Phys. Rev. B **91**, 224411 (2015); *eidem*, Phys. Rev. B **91**, 174409 (2015); [3] R. Chisnell et al., Phys. Rev. Lett. **115**, 147201 (2015); [4] Y. Onose et al., Science **329**, 297 (2010).

O 41.7 Tue 15:45 H24

Acoustic magnons in the long-wavelength limit: resolving the Goldstone violation in many-body perturbation theory — •Mathias C.T.D. Müller, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Ferromagnetic materials exhibit a spontaneously broken global rotation symmetry in spin space leading to the appearance of massless quasiparticles (zero gap) in the long-wavelength limit. These magnons are formed by the correlated motion of electron-hole pairs with opposite spins, which we describe from first principles employing the T-matrix formalism in the ladder approximation within the FLAPW method [1]. Due to approximations used in the numerical scheme, the acoustic magnon dispersion exhibits a small but finite gap at Γ. We analyze this violation of the Goldstone mode and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the Kohn-Sham (KS) one. This much more expensive approach shows substantial improvement of the Goldstone-mode condition. In addition, we discuss a possible correction scheme, that involves an adjustment of the KS exchange splitting, which is motivated by the spin-wave solution of the one-band Hubbard model. The new exchange splittings turn out to be closer to experiment. We present corrected magnon spectra for the elementary ferromagnets Fe, Co, and Ni.
[1] E. Şaşıoğlu *et al.*, Phys. Rev. B **81**, 054434 (2010); C. Friedrich *et al.* Top. Curr. Chem. **347**, 259 (2014).

O 42: Plasmonics and Nanooptics III: Infrared Microscopy

Time: Tuesday 14:00–16:00 Location: H4

O 42.1 Tue 14:00 H4

Determination of local variations in charge carrier concentrations of doped nanowires using infrared near-field microscopy — •Lena Jung[1], Robert Ukropec[1,2], Fabian Haas[2], Hilde Hardtdegen[2], Thomas Schäpers[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]Peter Grünberg Institut 9, Forschungszentrum Jülich, 52425 Jülich, Germany

In scattering-type scanning near-field optical microscopy (s-SNOM), optical near-fields are generated at the apex of a sharp illuminated tip. The near-fields interact with the part of the sample in close proximity to the tip, therefore the back-scattered light contains information about the optical properties of the sample with a resolution only limited by the sharpness of the tip. We use this high resolution for the investigation of local variations in the charge carrier density of doped semiconductor nanowires (NW). Since the SNOM signals are related to the dielectric function of the sample material, which in turn can be connected to charge carrier density and mobility for doped semiconductors by applying the Drude model, it is possible to determine these important quantities from the spectroscopic SNOM signals. Measurements on partly doped Si-NW will be presented as well as on contacted InAs-NW. With a sample holder that allows contacting the sample, which was specifically designed for this sample system, we were able to perform SNOM measurements of these NW by at the same time applying a source-drain voltage and a backgate to the nanowires. This allows for the investigation of the direct influence of gating on the NW.

O 42.2 Tue 14:15 H4

Experimental investigation of the depth-dependent near-field coupling in subsurface s-SNOM imaging. — •Mike Prämassing, Martin Lewin, and Thomas Taubner — Institute of Physics (IA) RWTH Aachen

Scattering-type Scanning Near-field Optical Microscopy (s-SNOM) is based on a laser-illuminated metal-coated tip being scanned over the sample. Due to the localized tip sample interaction, the optical properties of the sample can be analysed on the nm-scale. Since the tip probes high spatial frequencies, s-SNOM is capable of imaging buried structures via evanescent waves [1]. We could distinguish between amorphous and crystalline regions of AgInSbTe even below 100 *nm* of capping layer [2]. The found complex material contrasts can be explained by theoretical calculations taking into account the layered structure of the sample [3]. At the sample surface, the tip predominantly probes spatial frequencies in the range of the inverse tip radius. Here we investigate the tip-sample-coupling for different burying depth and spatial frequencies. High quality gold gratings are employed to produce well defined spatial frequencies. The Depth dependence of the coupling of the tip to these spatial frequencies is investigated by measuring the gratings buried below PMMA layers of varying thickness.

[1] Taubner et al., Opt. Express 13, 8893 (2005)
[2] Lewin et al., Appl. Phys. Lett., 107, 151902 (2015)
[3] Hauer et al., Opt Expr. 20, 13173 (2012)

O 42.3 Tue 14:30 H4

Amplitude-modulated scattering cross-section in near-field infrared microscopy (s-SNIM) — •Frederik Kuschewski[1], S.C. Kehr[1], N. Awari[2], B. Green[2], S. Kovalev[2], M. Gensch[2], and L.M. Eng[1] — [1]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institut für Strahlenphysik, 01314 Dresden, Germany

Scattering-type scanning near-field optical microscopy (s-SNIM) was applied to investigate the local infrared-optical properties of Ge, Si and SiGe thin films in a pump-probe experiment below the diffraction limit. The combination of s-SNIM with pump-probe techniques allows for studying electron-excitation processes at an ultimate temporal resolution, and for investigating their decay behavior.

Pump excitation is exhibited in our setup with different NIR laser systems, while near-field probing was carried out either by using a cw CO_2 or the tuneable free-electron-laser at the Helmholtz-Zentrum Dresden-Rossendorf. The periodic optical excitation of the sample induces sidebands to the higher-harmonics in our s-SNIM setup, that contain the pure pump-induced information [1]. Using a special demodulation technique, the existence of these new frequencies was proven up to the 10th sideband. The investigated samples show a time-variable pump-effect in the near-field when being probed at $\sim$10 μm wavelength. Image scans clearly proof the resolution far beyond the diffraction limit. Our experiment proves that ultra-fast phenomena may elegantly be probed in the near field with a superb sub-diffraction resolution.

[1] F. Kuschewski. et al., *Scientific Reports* **5**, 12582 (2015).

O 42.4 Tue 14:45 H4

Exploring local-scale phase transitions by low-temperature scattering scanning near-field optical microscopy — •Jonathan Döring, Susanne C. Kehr, and Lukas M. Eng — IAPP, Technische Universität Dresden

Using a low-temperature (T $\geq$ 4 K) scattering scanning near-field optical microscope (LT-s-SNOM) in conjunction with infrared photon excitation from a tunable free-electron laser (FEL) source, we are able to explore phase transitions in various systems down to the 1-nm length scale.

In LT-s-SNOM, the light scattered off an atomic force microscopy tip is strongly dependent on the tip-sample near-field interaction. Hence, recording this local light scattering enables imaging of optical properties with a resolution several orders of magnitude below the diffraction limit. The FEL laser light source provides high power densities and is precisely spectrally tunable from 4 to 250 μm. The unique combination of LT-s-SNOM and FEL thus allows for investigating a manifold of phonon-resonant phase transitions between 4 - 300 K by both nano-imaging and nano-spectroscopy. We report here on such studies for different systems; ferroelectric barium titanate [1] and doped lanthanum manganites [2]. Our LT near-field studies are backed-up by complementary piezo-response force microscopy (PFM) and Kelvin probe force microscopy (KPFM) performed in-situ with one and the same AFM.

[1] J. Döring et al., Appl. Phys. Lett. 105, 053109 (2014).

[2] E. Beyreuther et al., Phys. Rev. B 80, 075106 (2009).

O 42.5 Tue 15:00 H4

Characterization of Thin Organic Layers using Synchrotron-based nano-FTIR Spectroscopy with adapted Storage Ring Optics — •Peter Hermann[1], Arne Hoehl[1], Bernd Kästner[1], C. Magnus Johnson[2], Piotr Patoka[3], Georg Ulrich[3], Jörg Feikes[4], Markus Ries[4], Tobias Götsch[4], Burkhard Beckhoff[1], Eckart Rühl[3], and Gerhard Ulm[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), 10587 Berlin, Germany — [2]School of Chemical Science and Engineering, KTH, SE-100 44 Stockholm, Sweden — [3]Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin, 14195 Berlin, Germany — [4]Helmholtz-Zentrum Berlin (HZB), 12489 Berlin, Germany

Near-field techniques such as infrared scanning near-field optical microscopy (SNOM) and nano-FTIR spectroscopy enable imaging and spectroscopic characterization of samples at the nanoscale. However, the spectroscopic characterization of thin organic films and monolayers requires additionally highly stable radiation sources with a broad emission spectrum in the mid-IR range, e.g. thermal and synchrotron based sources. In order to exploit the full potential of this approach, we report on the adaption of storage ring optics at the Metrology Light Source (MLS). This results in a significantly reduced size of the electron bunches. In combination with appropriate spectral filters the sensitivity of synchrotron-based near-field spectroscopy can be increased even further, thus enabling also the spectroscopic characterization of organic samples. This is demonstrated by performing nano-FTIR spectroscopy and nano-imaging on biological model systems.

O 42.6 Tue 15:15 H4

Surface-enhanced infrared chemical imaging — •Frank Neubrech[1], Lucca Kühner[1], Mario Hentschel[1], Ute Zschieschang[2], Hagen Klauk[2], and Harald Giessen[1] — [1]4. Physics Institute and Research Center SCoPE, University Stuttgart, Stuttgart — [2]Max Planck Institute for Solid State Research, Stuttgart

Infrared (IR) chemical imaging provides laterally resolved spectroscopic information of molecular species based on their material-specific vibrational bands. Nowadays, this powerful method is applied in medicine and pharmacy to identify different drugs or to differentiate between healthy and diseased tissues. However, the method suffers from the relatively low excitation cross-sections of the IR vibrations. To overcome this limitation, we combine surface-enhanced infrared spectroscopy (SEIRA), which enables the detection of minute amounts of molecules down to attomolar concentrations, and chemical imaging to map heterogeneous molecular layers of nanometer thickness. More specifically, we evaporated 30 nm thick areas of pentacene as well as C_{60} using shadow mask lithography on highly homogeneous nanoantenna arrays fabricated by electron beam lithography. The acquired chemical maps demonstrate a significantly improved detection limit in comparison to conventional chemical imaging.

O 42.7 Tue 15:30 H4

Terahertz spectroscopy of individual donors in silicon by low temperature s-SNOM — •Denny Lang[1], Stephan Winnerl[1], Harald Schneider[1], Juerong Li[2], Steve Clowes[2], Ben Murdin[2], Jonathan Döring[3], Susanne C. Kehr[3], Lukas M. Eng[3], and Manfred Helm[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany. — [2]University of Surrey, Guildford, UK. — [3]Technische Universität Dresden, Germany.

Isolated atoms or ions, typically confined in traps, are ideal systems for studying fascinating coherent quantum effects such as photon echoes. Likewise, isolated donor impurity atoms in semiconductors like silicon show a hydrogen-like spectrum, shifted to the far infrared due to the small effective mass and high dielectric constant [1]. Excited Rydberg states are of particular interest for quantum information, because they allow one to prepare long-living microscopic polarization states.

In contrast to previous far-field spectroscopic studies which probed ensembles of many impurities, we aim here at studying individual impurity centers. To this end, low-temperature scattering-type scanning near-field optical microscopy (s-SNOM) is employed and a free-electron laser is used as a precisely tunable terahertz source [2]. Our silicon samples contain different donors (P, Bi) with different defect densities, respectively, and are pre-characterized by conventional Fourier transform infrared spectroscopy.

[1] Greenland et al., Nature 465, 1057 (2010).

[2] Döring et al., Appl. Phys. Lett. 105, 053109 (2014).

O 42.8 Tue 15:45 H4

Terahertz responses of a metal with sub-nm gap — •tae yun kim[1], sang jun park[1], dai-sik kim[2], and cheol-hwan park[1] — [1]Center for Theoretical Physics and Department of Physics, Seoul National University, Seoul 08826, Korea — [2]Center for Atomic Scale Electromagnetism and Department of Physics, Seoul National University, Seoul 08826, Korea

Recent developments have shown that the characteristic length scale of a plasmonic system can reach a few angstroms. In a recent experiment, it was observed that the tunneling of electrons through quantum barriers can restrict the funneling of terahertz waves through sub-nm gaps in the extremely non-linear, high-intensity regime [1]. In this contribution, we calculate and discuss the responses of a metal with sub-nm gaps in the terahertz regime further based on a recent theoretical study [2].

[1] Young-Mi Bahk, Bong Joo Kang, Yong Seung Kim, Joon-Yeon Kim, Won Tae Kim, Tae Yun Kim, Taehee Kang, Jiyeah Rhie, Sanghoon Han, Cheol-Hwan Park, Fabian Rotermund, and Dai-Sik Kim, Phys. Rev. Lett. 115, 125501 (2015).

[2] Sang Jun Park, Tae Yun Kim, Cheol-Hwan Park, and Dai-Sik Kim, unpublished.

O 43: Oxides and Insulators: Adsorption I

Time: Tuesday 14:00–16:00 Location: H6

O 43.1 Tue 14:00 H6

Dissociated but not separated: Adsorption of water at the SrO surface of ruthenates — •Florian Mittendorfer[1], Daniel Halwidl[1], Bernhard Stöger[1], Wernfried Mayr-Schmölzer[1], Jiri Pavelec[1], David Fobes[2], Jin Peng[2], Zhiqiang Mao[2], Gareth Parkinson[1], Michael Schmid[1], Josef Redinger[1], and Ulrike Diebold[1] — [1]Inst. of Applied Physics, TU Wien, Vienna, Austria — [2]Dept. of Physics, Tulane University, New Orleans, USA.

Despite their great promise in applications ranging from solid oxide fuel cells to catalysts, molecular level knowledge about the surface chemistry of perovskite oxides is surprisingly poor. To gain more insight, we follow the formation of the first monolayer of H_2O at the (001) surfaces of $Sr_{n+1}Ru_nO_{3n+1}$ (n=1,2) using low-temperature STM, XPS, and DFT. These layered perovskites cleave between neighbouring SrO planes, yielding almost ideal, rocksalt-like surfaces. An adsorbed monomer dissociates and forms a pair of hydroxide ions. The OH stemming from the original molecule stays trapped at Sr-Sr bridge positions, circling the surface OH with a measured activation energy of 187 ± 10 meV confirming almost perfectly the calculated DFT value of 171 meV [1]. At higher coverage, dimers of dissociated H_2O assemble into one-dimensional chains and form a percolating network where H_2O adsorbs molecularly in the gaps. Our work clearly shows that caution is needed when applying surface chemistry concepts derived for binary rocksalt oxides to perovskites.
[1] D. Halwidl et. al., Nature Materials, doi: 10.1038/nmat4512, 2015.

O 43.2 Tue 14:15 H6

Adsorption of water on the (001) surface of Fe3O4 studied by surface x-ray diffraction — •Björn Arndt[1,2], Heshmat Noei[1], Roland Bliem[3], Oscar Gamba[3], Gareth Parkinson[3], Ulrike Diebold[3], and Andreas Stierle[1,2] — [1]Deutsches Elektron-Synchrotron (Desy), D-22607 Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, D-20355 Hamburg, Germany — [3]Institute of Applied Physics, Vienna University of Technology, 1060 Vienna, Austria

Magnetite (Fe3O4) exhibits interesting properties which makes it attractive for applications e.g. in catalysis, where it is used to catalyze the water-gas shift reaction. The (001) surface of magnetite shows a (sqrt(2)x sqrt(2))R45° surface reconstruction in UHV [1], which gets lifted upon adsorption of water vapor at room temperature. Previous studies of the adsorption of water at different coverages on this surface were done by XPS measurements [2], without linking it to the surface structure. To probe the unreconstructed surface structure, we therefore performed surface x-ray diffraction at the ESRF ID03 beamline under flow conditions at a photon energy of 11 keV and at the MPG diffraction beamline at ANKA under static conditions at 10 keV and water vapor pressures in the mbar regime at room temperature. We were able to follow the lifting of the surface reconstruction and observed changes in the morphology of the surface. Crystal truncation rod data give insight into the surface structure. 1. Bliem et al., Science, 346, 1215-1218 (2014) 2. Kendelewicz, T. et al., J. Phys. Chem. C 117 , 2719-2733 (2013)

O 43.3 Tue 14:30 H6

Ab-initio simulations of water splitting on hematite — •Nicola Seriani — The Abdus Salam ICTP, Trieste, Italy

Hematite has recently raised considerable interest as a possible photocatalyst for water oxidation. Despite the on-going research efforts, its efficiency is still unsatisfactory. To understand the behaviour of hematite in a realistic environment, we have performed first-principles simulations based on density functional theory. By taking into account the presence of water and oxygen under illumination, we show that the thermodynamically stable surface termination under reaction conditions is oxygen rich. On this termination, water oxidation proceeds by nucleophilic attack with an overpotential of 0.84 V. Then, we have considered the possible effect of surface modifications such as impurities and ultrathin films on the properties of the surface. Nitrogen doping lowers the overpotential, while detrimental surface states disappear in presence of ultrathin films of gallium oxide or aluminium oxide. I am going to compare calculations with available experiments, and to discuss open questions and future developments in this field.

O 43.4 Tue 14:45 H6

Derivation and Validation of a Classical Potential for Surfaces of Ionic Crystals — •Sara Panahian Jand and Payam Kaghazchi — Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

In this work, we present a method to parametrize Coulomb+Buckingham (C-B) pairwise potentials that can be used to study the atomic structure and stability of surfaces of ionic crystals. Our training sets are based on density functional theory (DFT) calculations. In the parametrization procedure, ionic charges are calculated using electrostatic energies and then Buckingham parameters are fitted to reproduce energy changes versus atomic displacements and unit cell size in bulk. Although depending on the starting points different sets of parameters are obtained, only one set of them can qualitatively reproduce (DFT-calculated) atomic structure and stability of low-index surfaces of ionic crystals. We found that the constructed potentials can calculate relaxations and relative stabilities of higher-index surfaces in good agreement with experiments and DFT [1]. Most of electrode and (solid) electrolyte materials in Li-based batteries have ionic crystals. Therefore, the method discussed in the present work [2] can be applied to construct reliable classical potentials for these materials to study electrode/electrolyte interfaces in Li-based batteries.

[1] S. Panahian Jand and P. Kaghazchi, J. Phys.: Condens. Matter, 26, 262001 (2014)

[2] S. Panahian Jand and P. Kaghazchi, submitted

O 43.5 Tue 15:00 H6

UHV-IR spectroscopy study of carbon monoxide adsorption on ceria single crystal surfaces — •Chengwu Yang, Alexei Nefedov, Yuemin Wang, and Chrostof Wöll — Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

Ceria, one of the most easily reducible metal oxides, exhibits extraordinary reactivities in diverse catalytic processes. The importance of this material has triggered numerous experimental and theoretical studies, in particular aiming at elucidating the properties of oxygen vacancies. The studies on bulk single crystal surfaces, however, are still scarce.

On a novel apparatus combining a state-of-the-art FT-IR spectrometer with a dedicated UHV-chamber, we used carbon monoxide (CO) to probe regular sites and oxygen vacancies at surfaces of bulk CeO2(111), CeO2(110), and CeO2(100) single crystals. It was found that the vibrational frequency of C-O stretching mode strongly depends on facet orientations as well as the reduction of ceria surfaces. The assignment of the CO stretch frequency as determined by IR-spectroscopy was supported by ab-initio electronic structure calculations using density functional theory. The obtained results clearly indicate that the application of CO adsorption as a IR-probe is quite suitable for the determination of facet orientations as well as for probing surface oxygen vacancies and allows us to clarify the ambiguous assignments derived from previous powder and thin film data.

O 43.6 Tue 15:15 H6

An *ab initio* study of adsorption and defect formation energies at the surface of Ni-doped MgO – a catalyst for the Sabatier process — •Aliaksei Mazheika, Sergey Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Deutschland

We present an *ab initio* study of Ni_{Mg} defects in Ni-doped MgO - a promising material for the catalytic conversion of methane and CO_2. First, a fraction of exact exchange α in the hybrid DFT functional HSE06 is identified such that HSE(α) closely reproduces CCSD(T) formation energies of Ni_{Mg} in MgO bulk, as well as the adsorption energies of CO and H_2 at the surface defects, calculated with embedded cluster models. HSE($\alpha = 0.3$) is found to reproduce all the CCSD(T) results with deviations of at most 0.1 eV. Using this functional and periodic models, we calculate the formation energy dependence on the position of Ni_{Mg} (in the bulk, subsurface, at the (001) terrace, monolayer step and corner), and the influence of the defects on the adsorption energies of CO_2, CH_4, CO, and H_2. The presence of Ni_{Mg} at the surface is found to have a minor effect on the adsorption energies of CH_4 and CO_2, independent of the coordination of the adsorption site, whereas it increases the adsorption energy of CO and particularly H_2. The adsorption energy of CO_2 calculated with HSE($\alpha = 0.3$) plus the ab initio many-body van der Waals correction [1] is about 0.4 eV larger than the PBE adsorption energy. - [1] A. Tkatchenko et al. PRL. 108, 236402 (2012)

O 43.7 Tue 15:30 H6

Adsorption and reactivity of phthalic acid on MgO(100) thin films — •Quratulain Tariq, Matthias Franke, Daniel Wechsler, Michael Röckert, Liang Zhang, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany

The adsorption of functional organic species on oxide surfaces has importance in many areas of research, for example, in molecular electronics, photovoltaics and biomedical implants. In this work, we report on the adsorption of phthalic acid, a simple dicarboxylic acid, on MgO(100) thin films on Ag(100), as a model for the anchoring of large, functional organic entities such as porphyrins or fullerenes. Using high-resolution synchrotron radiation photoelectron spectroscopy (SRPES), near-edge X-ray absorption fine structure (NEXAFS) and temperature-programmed desorption (TPD), we find that the phthalic acid dissociates below 150 K to phthalic anhydride and carboxylate. Phthalic anhydride desorbs at around 240 K. Carboxylate binds to MgO as bis-bidendate species and stable up to 500 K, after which it decomposes, through desorption of CO2. This project is supported by the DFG through FOR 1878 (funCOS).

O 43.8 Tue 15:45 H6

Electrospray deposition of organic molecules in UHV on bulk insulator surfaces — •Antoine Hinaut, Rémy Pawlak, Thilo Glatzel, and Ernst Meyer — Department of Physic, University of Basel Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Adsorption of molecules, isolated or as assemblies, on surfaces under ultra high vacuum (UHV) conditions is an important field in nanoscience and lead to many applications such as photovoltaic, molecular electronic or surface functionalization. To study larger and more complex molecules in such conditions, suitable for such devices an alternative method to thermal evaporation is to use Electrospray ionisation system. In that way, the deposition of molecules contained in solution on atomically-clean surfaces is not limited to their size or their reactivity.

In our measurement we imaged, by bimodal non-contact atomic force microscopy (ncAFM), adsorbed molecules that were deposited on the bulk insulator surface KBr(001) via electrospray deposition. The molecule is a triply fused diporphyrin, which includes two zinc atoms and two di-cyanophenyl groups for a better anchoring on the KBr(001) surface. For large coverage we found charging of the surface due to the deposition. Comparison of the surface before and after the charge compensation will be presented. For lower coverage no charging effects were observed and single molecules have been imaged.

O 44: Graphene: Electronic Properties, Structure and Substrate Interaction

Time: Tuesday 18:15–20:30 Location: Poster E

O 44.1 Tue 18:15 Poster E

Effect of electron-density inhomogeneities on the electronic band structure of single-layer graphene — •Trevor Clarke[1,2], Peter Kot[1,2], Jon Parnell[1,2], Sina Habibian[1,2], Klaus Kern[1,3], and Christian R. Ast[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]University of British Columbia, Vancouver, Canada — [3]École Polytechnique Fédérale de Lausanne, Switzerland

In an ideal graphene sheet, the density of electrons is uniformly distributed throughout the two-dimensional lattice. However, in experimental contexts, graphene sheets are routinely subject to electron-density inhomogeneities. Such inhomogeneities, or charge puddles, are thought to arise from charged impurities located on the substrate on which the graphene is deposited. To investigate the effects of charge puddles on the electronic properties of single-layer graphene, we simulate fluctuating potential landscapes that model charge inhomogeneities via two methods: the diamond-square algorithm, and fractional Brownian motion (with Perlin noise). Each method produces randomly fluctuating (but smooth and continuous) potential landscapes with unique features and characteristics. These potential landscapes are used to perturb the on-site energies of the carbon atoms in the lattice. The band structure of the perturbed lattice is then calculated using a tight-binding model. We present calculations exploring a range of parameter values, and indicate results produced from values which generate potentials that most closely resemble empirical findings.

O 44.2 Tue 18:15 Poster E

Robust ballistic transport phenomena in epitaxial graphene nanoribbons — •Johannes Aprojanz, Jens Baringhaus, Maren Wehr, Felix Klösel, and Christoph Tegenkamp — Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany

Graphene nanoribbons (GNRs) are of particular importance for future carbon-based electronics. Their outstanding electronic properties, especially the presence of topologically protected ballistic transport channels, make them a prime candidate for a new class of fully coherent devices. However, the large amount of defects introduced by conventional lithography processes prevents the formation of such edge channels. The self-assembling growth of GNRs on the sidewalls of SiC mesa structures overcomes this obstacle leading to the observation of exceptional ballistic transport properties. With local transport experiments by means of a 4-tip STM, two fundamentally different ballistic modes can be identified. One is thermally activated and exhibits a mediocre mean free path in the order of several hundred nm, the other is temperature independent and shows an exceptionally long mean free path larger than $10\,\mu$m [1]. The roughness of the underlying SiC substrate is identified as a major source for electronic scattering. Consequently, the mean free path is shown to be directly dependent on the width of the substrate terraces [2].

[1] Baringhaus et al., Nature **506**, 349 (2014)
[2] Baringhaus et al., APL **106**, 043109 (2015)

O 44.3 Tue 18:15 Poster E

A bottom-up approach to synthesize graphene nanoribbons on Ru(0001) by chemical vapor deposition — •Ann-Kathrin Henss and Joost Wintterlin — Ludwig-Maximilians-Universität, Munich, Germany

The synthesis of defined graphene nanoribbons is of great interest for future applications due to their tunable band gaps. We have tested a bottom-up approach to synthesize graphene nanoribbons by chemical vapor deposition (CVD) of hydrocarbons on a prestructured Ru(0001) single crystal under ultra high vacuum conditions. The structuring of the substrate was achieved by aluminum deposition at elevated sample temperatures to decorate the step edges of the Ru(0001) surface. A subsequent oxidation step led to the formation of ordered stripes of aluminum oxide along the step edges which are to act as barriers between which graphene could grow in form of nanoribbons. Graphene was grown by CVD using ethylene as a precursor gas at 850°C and a pressure of 3×10^{-9} Torr. Scanning tunneling microscopy and Auger electron spectroscopy were used to monitor the synthesis steps. After the graphene growth no ordered structures of aluminum oxide were present on the surface anymore. Hydrogen forming during the decomposition of ethylene was found to reduce the aluminum oxide to metallic aluminum, which is no longer a growth barrier for graphene.

O 44.4 Tue 18:15 Poster E

Twisted graphene layers on metals investigated by scanning tunneling microscopy — •Sabina Simon, Philipp Leicht, Julia Tesch, Luca Gragnaniello, and Mikhail Fonin — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Epitaxial growth on metal substrates is known to be one of the most powerful approaches in producing large-scale high-quality monolayer graphene, yet it remains a major challenge to realize the growth of multilayers.

This work is devoted to the investigation of multilayered graphene systems epitaxially grown on metallic substrates. Firstly, we discuss the local electronic properties of twisted graphene flakes on Au(111). The electronic properties of such twisted bilayer graphene areas show an increased accessibility of atomically resolved graphene features, a shift of the Dirac energy closer to E_F with a residual doping of

85 meV and a reduced Fermi velocity of $(0.8\pm0.1)\cdot10^6$ m/s. Secondly, we present the results of the investigation of growth of large scale graphene bilayers on Ir(111) and report on their structure and electronic properties.

O 44.5 Tue 18:15 Poster E

Graphene formation on Ag(001) by liquid precursor deposition — •Jens Uwe Neurohr, Samuel Grandthyll, Karin Jacobs, and Frank Müller — Saarland University, 66041 Saarbruecken, Germany

Chemical vapor deposition (CVD) is the standard method for epitaxial growth of graphene on many transition metal surfaces, but for a very weakly interacting substrate such as Ag(001) the CVD-process fails. However, epitaxial graphene on Ag(001) can be obtained by liquid precursor deposition (LPD) - an alternative synthesis route that was successfully demonstrated on many transition metals in previous studies [1]. Graphene growth on Ag(001) was investigated by X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED), and Fermi surface mapping (FSM), revealing a monolayer coverage of arbitrarily rotated domains [2], similarly to the growth of boronitrene (i.e., h-BN monolayers) on the Ag(001) [3].

References:
[1] S. Grandthyll, S. Gsell, M. Weinl, M. Schreck, S. Hüfner and F. Müller J. Phys. : Condens. Matter 24 (2012) 314204
[2] S. Grandthyll, K. Jacobs and F. Müller Phys. Status Solidi B, 252: 1695-1699
[3] F. Müller, S. Grandthyll Surface Science 617 (2013) 207-210

O 44.6 Tue 18:15 Poster E

Lifting Graphene from Substrates by Scanning Tunneling Microscopy — •Anne Holtsch, Anne Holtsch, Wolf-Rüdiger Hannes, and Uwe Hartmann — Universität des Saarlandes, Saarbrücken

Graphene as a two-dimensional crystal is only stable because of the formation of so-called ripples. Such ripples are thus called intrinsic and have been identified both by transmission electron microscopy [1] and scanning tunneling microscopy (STM) [2].

Here we study graphene grown via CVD and transferred onto copper foils, which may cause corrugations either before, during or after transfer. We find, however, that the corrugations appear very similar to those of free-standing membranes [2]. We report on the lifting of the graphene from the copper substrates using the attractive forces of a STM tip as previously reported for graphene on silicon dioxide [3].

Since metallic substrates electronically bind to the adsorbing graphene, higher bias voltages for lifting are generally required than in the case of free-standing membranes. Other features of Z(V) spectroscopy curves such as reversible flipping processes with hysteric behavior are also analyzed. It is discussed wether interaction strengths between graphene and particular types of substrates can be deduced from such measurement.

[1] J. C. Meyer et al., Nature 446, 60 (2007) [2] R. Dan et al., Nanoscale 4, 3065 (2010) [3] T. Mashoff et al., Nano Lett. 10, 461 (2010)

O 44.7 Tue 18:15 Poster E

Flipping ripples of freestanding graphene membranes using Scanning Tunneling Microscopy — •Bernd Uder, Wolf-Rüdiger Hannes, and Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, Germany

Measurement and control of the elastic properties of two-dimensional materials is a prerequisite for their development into nanoelectromechanical systems. So far atomic force microscopy has been the only tool used to determine elastic moduli and breaking strength of freestanding graphene membranes [1]. This method usually does not allow a thorough characterization in terms of defect concentration and other sample parameters. Here we report on the deformation of graphene membranes using the attractive forces of a scanning tunneling microscope tip. The method poses challenges since membrane and tip instabilities are easily induced. We have been able to initiate flipping processes, which are reversible but show a hysteresis. Cascade like flipping and metastable membrane states are also observed. Possible relations with local elastic properties of the rippled membrane structure are discussed within a simple model.

[1] C. Lee, X. Wei, J. W. Kysar, J. Hone, Science 321, 385 (2008)

O 44.8 Tue 18:15 Poster E

Local transport measurements in Graphene on SiO2 using Kelvin Probe Force Microscopy — Philip Willke[1], Christian Möhle[1], •Anna Sinterhauf[1], Hak Ki Yu[2,3,4], Alec Wodtke[2,3], and Martin Wenderoth[1] — [1]IV. Physical Institute, University of Göttingen, 37077 Göttingen, Germany — [2]Institute for Physical Chemistry, University of Göttingen, 37077 Göttingen, Germany — [3]Max Planck Institute for Biophysical Chemistry, 37077 Göttingen, Germany — [4]Department of Materials Science & Engineering, Ajou University, Suwon 443-749, Korea

By using Kelvin Probe Force Microscopy with an additional applied electric field we investigate the local voltage drop in graphene on SiO2 under ambient conditions. We are able to quantify the variation of the local sheet resistance and to resolve localized voltage drops at line defects. Our data demonstrates that the resistance of line defects has been overestimated so far. Moreover, we show that different types of wrinkles have the largest resistance. Temperature-dependent measurements show that the local monolayer sheet resistance reflects the macroscopic increase in resistance with temperature while the defect resistance for folded wrinkles is best described by a temperature-independent model which we attribute to interlayer tunneling. This work was supported by the Deutsche Forschungsgemeinschaft (DFG) priority program 1459 Graphene.

O 44.9 Tue 18:15 Poster E

Epitaxial graphene via flash annealing of SiC studied by VT-STM — •Ismail Baltaci, Malte Schulte, Eugenia Wodopian, Harry Ritter, and Carsten Westphal — Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Strasse , 44227 Dortmund, Germany

Graphene has a charge carrier mobility which is two magnitudes larger than in SiC. Therefore graphene is of particular relevance for the semiconductor industry, e.g. as a new material for transistors.

There are different methods which should yield large and homogeneous graphene layers. Here we concentrate on an epitaxial growth based on cyclic heating of SiC, known as flash annealing. The hydrocarbon contaminations are desorbed during degasing SiC at 600° C. Heating up to 1400° C leads to a sublimation of Si. The remaining carbon atoms reconstruct in a hexagonal structure forming large graphene layers.

In addition to the flash annealing we are using hydrogen etching to achieve a high quality and flat SiC surface prior to the annealing steps. A Si- or Ar-flux during the annealing reduces the Si-sublimation and thus increases the graphene quality. In order to optimize the procedure multiple parameters have to be taken in account. Imaging the surface of SiC/Graphene is achieved by VT-STM.

O 44.10 Tue 18:15 Poster E

STM characterization of epitaxial graphene produced by confinement controlled sublimation of SiC — •Hermann Kromer[1], Cornelis Hilscher[1], Richard Hönig[1], Christoph Keutner[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund, Germany

Graphene electronics imposes great demands on the material and material processing. The realization of graphene-based electronics requires a homogeneous, controllable and reproducible growth of large-domain graphene layers.

In this study we are focusing on the growth of epitaxial graphene on the Si-face of silicon carbide (SiC). Our aim is to achieve a well controlled growth of high quality graphene layers on a large scale. Therefore we are using the confinement controlled sublimation (CCS) method under ultra high vacuum (UHV) conditions, as well as in an argon atmosphere.

After the preparation, these samples are characterized by scanning tunneling microscopy (STM). STM is an excellent tool to study this system, since its high resolution enables us to examine surfaces down to the atomic level.

O 44.11 Tue 18:15 Poster E

Graphene growth on SiC($11\bar{2}0$) — •Stefanie Rumbke, Florian Speck, and Thomas Seyller — Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany

Epitaxial growth of graphene on SiC(0001) surfaces leads to the formation of the so-called buffer layer, a monolayer of carbon atoms partially bonded to the substrate [1]. This layer is known to be detrimental for the electronic transport properties of graphene [2]. We present a study of graphene growth on SiC($11\bar{2}0$) surfaces on which, according to previous work [3], graphene can be grown on top of the substrate without a buffer layer residing at the interface. Prior to graphene growth, samples were hydrogen etched in order to obtain flat surfaces. Systematic studies were carried out to determine the optimal parameters for both hydrogen etching and graphene growth. For hydrogen etching temperature as well as hydrogen flow were varied, for graphene growth temperature and duration of the growth process. The quality of the hydrogen etched surfaces and the graphene layers along with the properties of the graphene were investigated using atomic force microscopy, x-ray photoelectron spectroscopy, low energy electron diffraction and angle-resolved photoelectron spectroscopy. In addition, the impact of hydrogen intercalation on the doping level of graphene on SiC($11\bar{2}0$) was investigated.

[1] K. Emtsev, et al., Phys. Rev. B **77**, 155303 (2008).
[2] F. Speck, et al., Appl. Phys. Lett. **99**, 122106 (2011).
[3] M. Ostler, et al., Phys. Rev. B **88**, 085408 (2013).

O 44.12 Tue 18:15 Poster E

High quality graphene on boron nitride prepared by polymer free dry transfer and contacting techniques for combined STM and electrical transport measurements — •Tjorven Johnsen, Daniel Montag, Felix Jekat, Martin Grob, Nils Freitag, Peter Nemes-Incze, and Markus Morgenstern — II. Physikalisches Institut B, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen

The charge carrier mobility of graphene is mainly determined by the substrate and adsorbates on the graphene flake. High quality graphene samples are prepared by either suspending the graphene flake or by encapsulating it in hexagonal boron nitride [1,2]. These devices, however, are not accessible for surface sensitive probes like scanning tunnelling microscopy (STM). Here we present a novel transfer technique employing a mica substrate to pick up a boron nitride flake and a graphene flake one after another from SiO_2. The graphene flake is contacted using shadow mask evaporation. Thereby, we eliminate any polymers from the preparation process which are a major source of adsorbates. This is required for combined STM and electrical transport measurements. With these samples we aim to measure symmetry broken states of the quantum hall effect in graphene both with STM and transport measurements.

[1]Du et al., Nat. Nanotechnol. 3, 491 - 495 (2008)
[2]Banszerus et al., Sci. Adv. 1, e1500222 (2015)

O 45: Graphene: Adsorption, Intercalation and Doping

Time: Tuesday 18:15–20:30 Location: Poster E

O 45.1 Tue 18:15 Poster E

Intercalation of epitaxial graphene on SiC by antimony — •Susanne Wolff[1], Sarah Roscher[1], Martina Wanke[1], Florian Speck[1], Christian Raidel[1], Marcus Daniel[2], Felix Timmermann[3], and Thomas Seyller[1] — [1]TU Chemnitz, Institut für Physik, Technische Physik, Germany — [2]TU Chemnitz, Institut für Physik, Oberflächen- und Grenzflächenphysik, Germany — [3]Universität Augsburg, Institut für Physik, Experimentalphysik IV, Germany

Graphene on SiC is grown epitaxially by sublimation growth. The first carbon layer grown is still covalently bound to the Si atoms of the substrate and therefore electronically inactive. Intercalation of epitaxial graphene on SiC decouples the buffer layer from the SiC substrate making it electronically active. In addition, intercalation can manipulate the structural and electronic properties. Thereby graphene can be adjusted for device applications.

In our x-ray photoelectron spectroscopy studies we investigated the intercalation of antimony on epitaxial graphene on SiC(0001). Antimony was evaporated from a Knudsen cell by molecular beam epitaxy at the surface and subsequently annealed with in a temperature range of 400°C to 500°C. Antimony shows different behavior for intercalation in ultra-high vacuum and argon atmosphere.

O 45.2 Tue 18:15 Poster E

Interaction of 10 nm-sized Co, Pd, and Ti islands with epitaxial graphene — •Anastasia Sokolova, Franziska Kilchert, and M.Alexander Schneider — Solid State Physics, Friedrich-Alexander University Erlangen-Nürnberg, Germany

We investigated the adsorption and intercalation properties of metals (Co, Pd and Ti) relevant for contact formation on epitaxial graphene on 6H-SiC(0001) by Scanning Tunneling Microscopy (STM).

When evaporated at substrate temperatures below 100°C, all three metals form (111) and (0001) oriented ad-islands. Only titanium showed a tendency to decorate substrate step edges. Judging from the cobalt and palladium ad-island stability with respect to material pick up by the STM tip, palladium forms weaker bonds to graphene than cobalt. Titanium ad-islands could also be removed by the STM tip. However we observe in the majority of cases that the graphene underneath is removed. We take this as an indication of a strong chemical interaction between titanium and graphene.

After annealing to approximately 600°C Co and Pd readily intercalate while Ti does not. Co intercalates by forming metal islands below the graphene sheet similar in size as the previous ad-islands, while Pd additionally formed large ($>$ 50 nm in lateral size) patches growing from step edges or holes in the graphene sheet indicating coalescence of intercalated material.

O 45.3 Tue 18:15 Poster E

Crystalline Xe underneath a monolayer of hexagonal boron nitride — •Philipp Valerius[1], Charlotte Herbig[1], Mohammad Alif Arman[2], Jan Knudsen[2,3], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Division of Synchrotron Radiation Research, Lund University, Box 118, 22100 Lund, Sweden — [3]MAX IV Laboratory, Lund University, Box 118, 22100 Lund, Sweden

Exposing a monolayer of hexagonal boron nitride on Ir(111) at room temperature to Xe irradiation in the energy range from a few 100 eV to a few 1000 eV causes amorphization of the 2D layer material, as shown by low energy electron diffraction. Surprisingly, upon annealing the hexagonal boron nitride recovers to perfection, except of vacancy islands resulting from sputtering and blisters formed due to aggregation of implanted species. With scanning tunneling microscopy we image through the hexagonal boron nitride blister lid and find a superstructure corresponding in lattice parameter to what we expect for a crystalline Xe layer. X-ray photoelectron spectroscopy experiments confirm this interpretation. We conclude that due to the strong adhesion of hexagonal boron nitride to Ir(111) the pressure inside the blisters is in the GPa range. An additional peculiar feature of our experiments are noble gas filled hexagonal boron nitride blisters, which are surrounded only by bare Ir(111).

O 45.4 Tue 18:15 Poster E

Band gap engineering by Bi intercalation of graphene on Ir(111) — •Jonas Warmuth[1], Matteo Michiardi[2], Albert Bruix Fusté[2], Torben Hänke[1], Marco Bianchi[2], Jens Wiebe[1], Roland Wiesendanger[1], Bjørk Hammer[2], Philip Hofmann[2], and Alexander Ako Khajetoorians[3,2] — [1]Dept. of Physics, Hamburg University, Hamburg, Germany — [2]Interdisciplinary Nanoscience Center and Department of Physics and Astronomy, Aarhus University, Denmark — [3]Institute of Molecules and Materials, Radboud University, Nijmegen, Netherlands

We report on the structural and electronic properties of a single bismuth layer intercalated underneath a graphene layer grown on an Ir(111) single crystal. Scanning tunneling microscopy (STM) reveals a hexagonal surface structure and a dislocation network upon Bi intercalation, which we attribute to a $\sqrt{3} \times \sqrt{3}$R30° Bi reconstruction on the underlying Ir(111) surface. Ab-initio calculations show that this Bi reconstruction is the most energetically favorable, and also illustrate that STM measurements are most sensitive to C atoms in close proximity to intercalated Bi atoms. Additionally, Bi intercalation induces a band gap (E_g = 0.42eV) at the Dirac point of graphene and an overall n-doping (0.39eV), as seen in angular-resolved photoemission spectroscopy. We attribute the emergence of the band gap to the dislocation network which forms favorably along certain parts of the moiré structure induced by the graphene/Ir(111) interface.

O 45.5 Tue 18:15 Poster E

Superstructures and Phonons of Graphene on Ir(111) Induced by Li Intercalation — •Johannes Halle, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

Lithium-intercalated graphene on Ir(111) exhibits various superstructures with increasing coverages as unveiled with low-temperature scanning tunnelling microscopy. At low coverages Li always resides at one specific high-symmetry site of the moiré pattern. Compact, elongated and trefoil-like Li clusters become the building blocks of superstructures at higher coverages. Their shapes and orientations reflect local strain variations in the graphene sheet and the energy landscape of different sites in the moiré unit cell. Intercalation of Li enables the observation of graphene phonons in inelastic electron tunnelling spectroscopy. While for pristine graphene phonon features stay below the detection limit, clear signatures of M point acoustic and optical phonons appear in the spectra of Li-intercalated graphene.

Funding by the Deutsche Forschungsgemeinschaft through KR 2912/10-1 is acknowledged.

O 45.6 Tue 18:15 Poster E

Near-Saturated Hydrogenation of Graphene on Ir(111) — •Clifford Murray, Ulrike Schröder, Antonio Martínez-Galera, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Hydrogen adsorption structures on graphene on Ir(111) have previously demonstrated their potential to modify the electronic properties of graphene (Gr) [1,2]. We have combined temperature programmed desorption (TPD) and scanning tunneling microscopy to further the understanding of this hydrogenation when close to saturation. We investigate dosage dependence of deuterium radical adsorption, diffusion thereof, and calculate coverages by calibrating TPD spectra. These spectra show two broad desorption peaks - at roughly 380K and 730K - representing two different adsorption states for deuterium on graphene. By growth of a Pt cluster superlattice we selectively block a specific area in the Gr moiré from adsorption. Subsequent radical exposure and the attenuation of the high temperature peak in desorption from this sample allows us to pin-point the binding area of the radicals. It is consistent with the formation of graphane-like patches in the moiré unit cell. We will speculate on the nature of the low temperature desorption peak.

[1] R. Balog et al., Nature Mater, 9, 315 (2010)

[2] R. Balog et al., ACS Nano, 7, 3823 (2013)

O 45.7 Tue 18:15 Poster E

Adsorption of molecules on graphene-supported iridium clusters — •Andreas Stoll, Kira Jochmann, and Thorsten Bernhardt — Universität Ulm

The adsorption of organosulfur and porphyrin molecules onto numerous metal and semiconductor substrates results in the formation of dense highly oriented self-assembled monolayer structures. Hitherto, the majority of studies dealt with the adsorption of these molecules on the Au(111) surface or on gold clusters in solution. In this contribution we investigate the adsorption of various organosulfur and prophyrin molecules on iridium clusters that were prepared on the moiré-type superstructure of graphene on Ir(111) by a combination of two photon photoemission spectroscopy and scanning tunneling microscopy (STM). The selection of this system was guided by the prospect to directly map the single chemisorbed molecules via room temperature STM. All molecules were found to exhibit unique geometric adsorption patterns on the bare Ir(111) surface, on graphene, and on the Ir clusters on graphene, respectively.

O 45.8 Tue 18:15 Poster E

Square ice sandwiched in graphene: a theoretical NMR study — •Achraf Jaadouni, Eva Rauls, Wolf Gero Schmidt, and Uwe Gerstmann — Uni Paderborn, Theoretische Physik, Pohlweg 55, 33100 Paderborn

Bulk water can exist in many forms, liquid, vapour and at least 16 crystalline phases, including the famous hexagonal ice [1]. Theory suggests, that many further phases can occur, if water is adsorbed on surfaces or confined on nanoscopic pores. A determination of the microscopic structure, however, provides a major challenge for experiment. Recently, locked between two graphene sheets, a new high-density phase has been observed by transmission electron microscopy (TEM) [2]. The so-called 'square ice' provides a symmetry qualitatively different from both hexagonal ice as well as graphene.

Modelling bilayer and trilayer lattices within density functional theory (DFT), we show that the phase transition from hexagonal to square ice is accompanied by a characteristic change of the NMR chemical shifts for the included protons. Hence, the detection via NMR spectroscopy appears as a promising alternative to electron imaging, in particular in case of nanostructures with a high amount of disorder, e.g. hydrophobic nanocapillaries.

[1] G. Malenkov, J. Phys. Condens. Matter 21, 283101 (2009).

[2] G. Algara-Siller et al., Nature 519, 443 (2015).

O 45.9 Tue 18:15 Poster E

Long range structure of oxygen and hydrogen adsorbed graphene — •Jan Gesenhues and Michael Rohlfing — WWU Münster

Adsorbtion of atomic oxygen and hydrogen on planar graphene is theoretically studied within a DFT-LDA framework. Changes in the spatial as well as electronic structure are studied in comparison to pristine graphene. In particular large supercells are considered to determine the long range effects of the respective adsorption. Our results show that the atomic adsorption mediates geometric changes as far as 20 Å while electronic changes can be observed approximately within 15 Å.

O 45.10 Tue 18:15 Poster E

Trends in chemical reactivity of carbon allotropes — •Sebastian Gsänger and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

The specific geometry of fullerenes, carbon nanotubes with different chirality and graphene imposes certain restrictions on the network of distributed π-bonds and therefore on their electronic properties and their reactivity towards adsorption. Using density-functional theory calculations, the adsorption energies of various adsorbates on the different allotropes was evaluated. For hydroxyl groups, adsorption patterns were analyzed and correlated with the electronic structure of the carbon allotrope. Finally, differences and similarities between the allotropes were identified and analyzed.

O 45.11 Tue 18:15 Poster E

Higher Order Corrected Spectroscopy at the Carbon K Edge — •Christine Jansing[1], Hans-Christoph Mertins[1], Andreas Gaupp[1,2], Andrey Sokolov[2], Markus Gilbert[1], Andreas Schümmer[1], Hud Wahab[3], Heiko Timmers[3], and Suk-Ho Choi[4] — [1]Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — [2]HZB, Albert Einstein Str. 15, D-12489 Berlin — [3]University of New South Wales, Canberra, ACT 2600, Australia — [4]Kyung Hee University, Yongin 446-701, Korea

We present the experimental determination of disturbing higher order synchrotron radiation across the carbon K edge at a soft x-ray beamline and a procedure to correct spectra of carbonaceous materials like highly oriented pyrolytic graphite (HOPG) or graphene. Measurements in the soft x-ray regime suffer from an enormous loss of photon flux at the C K edge, caused by carbon contamination of the beamlines optical elements. The unavoidable contaminations result from residual organic molecules in the beamline getting cracked by synchrotron radiation and absorbed as adventious carbon on mirrors. In particular first order radiation is absorbed so that incident light has large contributions from higher order wavelengths. We determined the amount of higher order light of up to 60% in the π^*-resonance of carbon exploiting a second monochromator and alternatively using a simple filter. We show that both methods reveal a reliable set of data to correct on higher order distortion of our experimental reflection and absorption spectra. This correction procedure can be applied to any carbonaceous material's spectra.

O 46: 2D Materials beyond Graphene: TMDCs, Slicene and Relatives

Time: Tuesday 18:15–20:30 Location: Poster E

O 46.1 Tue 18:15 Poster E

Growth and Characterization of Thin MoS_2 Films on the Buffer Layer on SiC(0001) — •Adrian Schütze[1], Martina Wanke[1], Florian Speck[1], Ovidiu Gordan[2], Gregor Nordheim[1], Thomas Seyller[1], and Dietrich R. T. Zahn[2] — [1]Professur für Technische Physik, TU Chemnitz, Germany — [2]Professur für Halbleiterphysik, TU Chemnitz, Germany

Layered 2D metal dichalcogenides such as MoS_2 are semiconductors with the unique property to transform from an indirect to a direct semiconductor depending on the number of layers. As such they are offering new possibilities for electronic applications. In this work, we study the large-scale chemical vapor deposition of thin layers of MoS_2 on the so-called buffer layer on SiC(0001), a graphene-like reconstruction with covalent bonds to the SiC substrate [1]. The buffer layer was grown in Ar at atmospheric pressure as described elsewhere [2]. MoS_2 was synthesized from $MoCl_5$ and sulfur powder [3] with Ar as carrier gas. X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM) and low-energy electron diffraction were used to characterize the chemical composition and structure of the samples. The thickness of the deposited MoS_2 is estimated to approximately 2 or 3 monolayers from XPS spectra and compared to Raman spectroscopy and AFM results. In addition, XPS data suggesting sulfur intercalation of the buffer layer during the CVD process are presented.

[1] K.V. Emtsev et al., Phys. Rev. B **77**, 155303 (2008).
[2] M. Ostler et al., Phys. Status Solidi B **247**, 2924 (2010).
[3] Y. Yu et al., Sci. Rep. **3**, 1866 (2013).

O 46.2 Tue 18:15 Poster E

Characterization of few layer MoS_2 on Silicon Carbide with Raman Spectroscopy — •Lisa Seitz[1], Adrian Schütze[2], Gregor Nordheim[2], Thomas Seyller[2], and Martin Hundhausen[1] — [1]Lehrstuhl für Laserphysik, FAU Erlangen-Nürnberg — [2]Professur für Technische Physik, Technische Universität Chemnitz

MoS_2 is a layered crystal with electronic properties that depend significantly on the number of layers. Here, we employ Raman spectroscopy for a mapping of layer number and homogeneity of few layer MoS_2, synthesized by CVD on silicon carbide (SiC). The frequencies of the E^1_{2g} and A_{1g} phonon modes depend on the layer number, so that the difference between these frequencies can be used as an indicator of layer number. [1] Different samples were studied by a Raman mapping: One sample shows a domain structure of terraces covered with bi- and trilayer MoS_2, coexisting with clean surface domains. Another sample shows a rather homogeneous coverage of MoS_2 with a layer number of around four to five.

[1] J. Jeon et al., Nanoscale **7**, 1688 (2015).

O 46.3 Tue 18:15 Poster E

Raman- and Photoluminescence Spectroscopy on few- and monolayered WSe_2 — •Walter Enns[1], Sergej Neb[1], Sebastian Fiechter[2], and Walter Pfeiffer[1] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Helmholtz Zentrum Berlin, Institut für Solare Brennstoffe, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The transition-metal dichalcogenide WSe_2 was exfoliated onto thermal oxidized silicon with 70 nm oxide thickness. Few- and monolayered flakes were investigated with confocal micro-Raman spectroscopy and photoluminescence spectroscopy applying two different wavelengths, 473 nm and 633 nm. The former measures the layer-dependent frequency difference of the out-of-plane to the in-plane vibration, while the latter is sensitive to the typical transition from indirect to direct band gap when changing from few-layer to monolayer WSe_2. Thus, both methods have the capability to distinguish between varying numbers of layers.

O 46.4 Tue 18:15 Poster E

Single-Layer MoS2 on Au(111): Electronic structure — Albert Bruix[1], Jill A. Miwa[1], •Nadine Hauptmann[2], Søren Ulstrup[1], Signe G. Grønborg[1], Charlotte E. Sanders[1], Maciej Dendzik[1], Antonija Grubišić Čabo[1], Marco Bianchi[1], Jeppe Vang Lauritsen[1], Daniel Wegner[2], Alexander A. Khajetoorians[2], Bjørk Hammer[1], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark — [2]Institute for Molecules and Materials, Radboud University, 6500 GL Nijmegen, The Netherlands

Single layer transition metal dichalcogenides are currently of considerable interest because they are 2D materials, like graphene, but have an inherent band gap. Their physical properties, e.g. their band gap and electronic structure, change dramatically in the single layer limit and depend on the underlying substrate. Molybdenum disulfide (MoS_2) as a single layer has already been used in applications such as field effect transistors and optoelectronic devices. We investigate epitaxial single-layer MoS_2 grown on Au(111) by low temperature scanning tunneling microscopy. Using scanning tunneling spectroscopy, we determine the single-particle band gap and compare it to density functional theory calculations of the electronic structure around the Fermi energy in the filled and empty states. At small energies, a low conductance regime is found while for higher energies onsets in the conductance are observed. These onsets are further compared to angle-resolved photoemission spectroscopy data from the same sample.

O 46.5 Tue 18:15 Poster E

Structure and Electronic Properties of MoS_2 on Au(111) — •Nils Krane, Christian Lotze, Julia Läger, Gaël Reecht, and Katharina J. Franke — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMCD) are two-dimensional materials with a natural band gap, making them interesting as sensors, solar cells or LEDs. Single layer molybdenum disulfide is especially interesting, because it provides a direct band gap [1] and a strong spin-splitting of the valence and conduction band.

Here we grow MoS_2 epitaxially on a Au(111) surface as described in [2]. Using a combined STM/AFM at low temperatures, we observe different kinds of defects. Particularly prominent are defects, which appear in sizes of several nanometers. The AFM reveals an atomically intact surface layer, suggesting that the origin of the defect is located at the gold interface. At these sites the bandgap of MoS_2 is significantly modified.

[1] Mak *et al.*, PRL 105, 136805 (2010)
[2] Sorensen, et al., ACS Nano 8, 6788-6796 2014

O 46.6 Tue 18:15 Poster E

Monolayer epitaxial hexagonal boron nitride on Ir(111) functionalization by caesium adsorption and intercalation — •Jiaqi Cai[1,2], Wouter Jolie[2], Caio Silva[1], Christoph Schlueter[3], Marin Petrovic[3], Marko Kralj[4], Tien-Lin Lee[4], and Carsten Busse[1,2] — [1]Institut für Materialphysik, Münster, Germany — [2]II. Physikalisches Institut, Köln, Germany — [3]Diamond Light Source Ltd, Didcot, United Kingdom — [4]Institut za fiziku, Zagreb, Croatia

Being a wide band gap insulator, hexagonal boron nitride monolayer (hBN) is an important member of the two-dimensional-material family. However, detailed information on the band structure remains unclear. In this respect, adsorption and intercalation of alkali metal on epitaxial hBN are easy routes to investigate its electronic structure.

Here, we report our study on caesium deposition on hBN/Ir(111). Scanning tunneling microscopy/spectroscopy (STM/STS), x-ray photoelectron spectroscopy (XPS), x-ray standing waves (XSW), and angle-resolved photoemission spectroscopy (ARPES) techniques are used to study the morphological and electronic properties of the system. The density and location of caesium (intercalated or adsorbed) varies when different deposition conditions are applied. Accordingly, different shifts of the hBN electronic bands occur in different caesium configurations. The largest shift towards higher binding energy obtained is 3.63 eV. Meanwhile no sign of the conduction band is observed in the ARPES results. This shows hBN has a band gap larger than 5.95 eV.

O 46.7 Tue 18:15 Poster E

Structural Analysis of one monolayer hBN on Cu(111) via SPA-LEED and NIXSW — •Christine Brülke[1], Niklas Humberg[1], Timo Heepenstrick[1], Ina Krieger[1], Simon Weiss[2], Sergey Subach[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52452 Jülich, Germany

Thin films of hexagonal boron nitride (hBN) are of high interest as an insulating material as well as a template for the formation of highly defined structures of organic molecules. Here, we report a detailed structural analysis of the hBN monolayer on the Cu(111) surface by spot profile analysis low energy electron diffraction (SPA-LEED) and normal incidence x-ray standing waves (NIXSW). hBN grows on the Cu(111) surface in an incommensurate structure with a lattice mismatch of 2.3 % corresponding to an unstrained hBN layer and a domain size of up to 170 Å. The films show rotational mosaicity, however, the majority of the hBN domains are in or close to alignment with the unit cell vectors of the Cu(111) surface. The highly resolved SPA-LEED patterns show detailed structures which can be explained entirely by multiple electron scattering. Both SPA-LEED and NIXSW experiments show that the hBN layer lies topologically flat on the copper surface. The average distance between adsorbate atoms and the first Cu layer is 3.24 ± 0.01 Å. We discuss our results in relation to previous studies.

O 46.8 Tue 18:15 Poster E

Hydrogenation and dehydrogenation of hexagonal - Boron Nitride (h-BN) on Ni(111) — •Florian Späth, Fabian Düll, Christoph Gleichweit, Udo Bauer, Philipp Bachmann, Christian Papp, and Hans-Peter Steinrück — Friedrich-Alexander-Universität, Erlangen-Nürnberg, Germany

Hexagonal-Boron Nitride (h-BN), which is a single atom thick sheet of alternatingly, hexagonal-arranged boron and nitrogen atoms, may be a suitable candidate for future hydrogen storage applications. Here, we investigate its reactivity towards atomic hydrogen, i.e. the hydrogenation, and subsequently the thermally activated dehydrogenation. The system is investigated with high-resolution temperature programmed X-ray photoelectron spectroscopy (HR-XPS) and temperature programmed desorption (TPD). h-BN is prepared via chemical vapor deposition of Borazine (B3N3H6) on a Ni(111) single crystal and subsequently exposed to atomic hydrogen at low temperatures. In HR-XPS, we find distinct chemical shifts after exposure to atomic hydrogen. In the temperature programmed investigation, we observe different dehydrogenation steps occurring at different temperatures, which depend on the initial hydrogen coverage. A comparison to the hydrogenation of graphene on Ni(111) will be shown. We acknowledge the support by the Cluster of Excellence "EAM" and the SFB 953 "Synthetic Carbon Allotropes".

O 46.9 Tue 18:15 Poster E

Epitaxial growth of Sn on SiC(0001): A study by scanning tunneling microscopy — •Felix Reis, Maximilian Bauernfeind, Ralph Claessen, and Jörg Schäfer — Physikalisches Institut, Universität Würzburg

This work is motivated by the unusual properties of graphene, which was the first material predicted to show the quantum spin Hall effect based on its spin-polarized topological edge states, which are located in the bulk energy gap. However, this gap is very small (order of μeV), such that it is impossible to access the edge channels in experiment.

One approach to overcome this problem is to pursue the realization of honeycomb lattices with high-Z atoms. A material that received great attention by theoretical modeling is (free-standing) stanene, made of Sn atoms and predicted to have a significantly larger bandgap due to stronger spin-orbit interaction [1]. However, a substrate – as needed for real-world experiments – had not been considered.

Here we report on the epitaxial growth of Sn reconstructions on SiC(0001) in the regime of around one monolayer coverage. The structures are examined by scanning tunneling microscopy (STM) and low-energy electron diffraction. We observe the formation of long-range ordered Sn-induced atomic lattices. Interestingly, depending on the coverage, these exhibit (3×3) or $(6\sqrt{3} \times \sqrt{3})$ superstructures, respectively. Close-up inspection is suggestive of hexagonal structural units. We will present a detailed analysis of the STM results, and discuss these in the light of theoretical predictions.

[1] Y. Xu *et al.*, Phys. Rev. Lett. **111**, 136804 (2013).

O 46.10 Tue 18:15 Poster E

Synthesis and Electronic Structure of Single-Crystal FeSe on Bi$_2$Se$_3$ — •Charlotte Sanders[1], Nils Rollfing[2], Andreas Eich[2], Fabian Arnold[1], Pascal Ewen[2], Marco Bianchi[1], Maciej Dendzik[1], Matteo Michiardi[1], Daniel Wegner[2], Philip Hofmann[1], and Alexander Ako Khajetoorians[2] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark — [2]Institute for Molecules and Materials, Radboud University, 6500 GL Nijmegen, Netherlands

Single-layer FeSe on SrTiO$_3$ exhibits a superconducting transition temperature T_c that is greatly enhanced over that of bulk FeSe. This fact—which is due, in part, to complex physics at the interface of these two materials—raises the question of whether interesting effects can be realised at the interfaces between FeSe and other types of substrates. Recent work has begun to elucidate the structure and electronic properties of single-crystal FeSe islands grown on the topological insulator Bi$_2$Se$_3$. Here we extend this line of investigation, combining scanning tunnelling microscopy and low-energy electron diffraction with a detailed mapping of the band structure using angle-resolved photoemission spectroscopy. Remarkably, our findings indicate persistence of the Dirac cone at the FeSe-Bi$_2$Se$_3$ interface. We do not observe superconductivity at temperatures down to 4.7K.

O 46.11 Tue 18:15 Poster E

Photoelectron Spectroscopy On Ferecrystalline Compounds — •Fabian Göhler[1], Gavin Mitchson[2], Matti Alemayehu[2], Christian Raidel[1], Florian Speck[1], David C. Johnson[2], and Thomas Seyller[1] — [1]Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany — [2]Department of Chemistry and Materials Science Institute, University of Oregon, Eugene, Oregon 97403, United States

Ever since the groundbreaking work on graphene by Novoselov and Geim, the preparation and properties of 2D materials have been of great interest to scientists. Going forward, the stacking of different sheet-like materials opens up new ways to design materials with specific properties. Recently, a new class of layered intergrowth materials built up from metal monochalcogenides and transition metal dichalcogenides has been prepared by the method of modulated elemental reactants (MER)[1]. These intergrowths have been termed *ferecrystals*[2], due to the turbostratic disorder occuring between the otherwise perfectly stacked layers.

Herein, we report the results of X-ray photoelectron spectroscopy studies carried out on (MSe)$_1$(NbSe$_2$)$_2$ ferecrystals, where M = Pb, Sn or Bi. Core level and valence band spectra of ferecrystals are compared to the MER-produced binary compounds of MSe and NbSe$_2$, respectively, to investigate inter-layer charge transfer in the ferecrystals.

[1] D. C. Johnson, *Curr. Opin. Solid State Mater. Sci.* **3**, 159 (1998).
[2] M. Beekman et al, *Semicond. Sci. Technol.* **29**, 064012 (2014).

O 46.12 Tue 18:15 Poster E

Angle-resolved photoemission spectroscopy of the possible chiral charge-density-wave state of $1T$-TiSe$_2$ — •Sascha Beier, Matthias Kallaene, Arndt Quer, and Kai Rossnagel — Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany

The layered transition-metal dichalcogenide $1T$-TiSe$_2$ undergoes a transition into a commensurate $2 \times 2 \times 2$ triple-q charge-density-wave (CDW) state at a temperature of ≈ 200 K. Recently, Ishioka *et al.* discovered a possible chiral CDW phase employing scanning tunneling microscopy (STM) below 85 K. Castellan *et al.* determined the transition temperature to this chiral CDW phase to be 7 K below the transition temperature into the normal CDW phase by specific heat, electrical transport properties, and X-ray diffraction measurements. However, a recent STM study questions the existence of an intrinsically chiral CDW state. Novello *et al.* rather attribute the effect to native lattice defects and the substitution of atoms.

Here we present angle-resolved photoelectron spectroscopy (ARPES) data on $1T$-TiSe$_2$ utilizing circular polarized synchrotron radiation. In the CDW phase, the electronic structure is characterized by a strong backfolding of the Se $4p$-derived bands to the L-point. Dichroism ARPES measurements of this spectroscopic order parameter at the L point apper to be consistent with the emergence of a chiral CDW state at temperatures below 190 K, in good agreement with the results of Castellan *et al.*

O 47: Electronic Structure of Surfaces: Spectroscopy, Surface States

Time: Tuesday 18:15–20:30 Location: Poster E

O 47.1 Tue 18:15 Poster E

Step and terrace conductivity of Ag/Si(111)-($\sqrt{3}\times\sqrt{3}$) and Si(111)-(7×7) measured by scanning tunneling potentiometry — •Felix Lüpke, Stefan Korte, Vasily Cherepanov, and Bert Voigtländer — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

We investigate the local electric potential of Ag($\sqrt{3}\times\sqrt{3}$) and (7×7) reconstructed Si(111) surfaces by means of scanning tunneling potentiometry: Two tips of a multi-tip scanning tunneling microscope inject a lateral current into the sample under investigation while a third tip is scanned across the sample surface measuring the topography and local potential simultaneously. From the measured sample geometry and potential distribution on its surface we extract surface and step conductivities.

O 47.2 Tue 18:15 Poster E

Local Tunneling Decay Length and Kelvin Probe Force Spectroscopy — •Florian Albrecht[1], Martin Fleischmann[2], Manfred Scheer[2], Leo Gross[3], and Jascha Repp[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Inorganic Chemistry, University of Regensburg, 93053 Regensburg, Germany — [3]IBM Research - Zurich, 8803 Rüschlikon, Switzerland

Current-distance spectroscopy has been widely applied to determine variations of the work function at surfaces. While for homogeneous sample areas this technique is commonly accepted to yield at least qualitative results, its applicability to atomic-scale variations has not been proven neither right nor wrong. Here we benchmark current-distance decay constant measurements against the well established Kelvin probe force spectroscopy method for distinctly different cases with atomic-scale variations of the local contact potential. Whereas the maps of the current-distance decay constant are consistent with being topographical artifacts, the Kelvin probe force spectroscopy maps show variations of the local contact potential difference in agreement with expected surface dipoles. This comparison clarifies that maps of the current-distance decay constant are not suited to directly characterize contact potential variations at surfaces on atomic length scales.

O 47.3 Tue 18:15 Poster E

Force and Kelvin Probe Measurements on Confined Electronic States inside Quantum Resonators — •Fabian Queck, Florian Albrecht, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

On close-packed surfaces of noble metals such as Cu(111) surface state electrons form a nearly free electron gas in two dimensions. The electrons are scattered from step-edges, point defects and adsorbates giving rise to standing wave patterns, which can be engineered by so-called quantum corrals (1). The standing wave patterns give rise to long range interactions between adsorbates (2) and should therefore be associated with measurable forces between scatterers.

At last year*s DPG meeting we presented preliminary results to directly measure these forces with atomic force microscopy and possible changes of the local contact potential difference arising from the modulation of the surface local density of states associated with the standing wave patterns. Here, we will present much more detailed atomic force microscopy and Kelvin probe spectroscopy data on this topic as well as electron density simulations that confirm our results.

(1) M. F. Crommie, C. P. Lutz, and D. M. Eigler. Confinement of Electrons to Quantum Corrals on a Metal Surface. Science, 262(5131):218*220, 1993.

(2) J. Repp. Rastertunnelmikroskopie und -spektroskopie an Adsorbaten auf Metall und Isolatoroberflaechen. PhD thesis, Freie Universitaet Berlin, 2002.

O 47.4 Tue 18:15 Poster E

Long-Lived Excited States in Porphyrin Nanostructures — •Hannes Hartmann[1], Ingo Barke[1], Alexej Friedrich[1], Per-Arno Plötz[1], Kevin Oldenburg[1], Johannes A.A.W. Elemans[2], Mohammadreza Bahrami[1], Karl-Heinz Meiwes-Broer[1], Oliver Kühn[1], Stefan Lochbrunner[1], and Sylvia Speller[1] — [1]University of Rostock, Institute of Physics, 18059 Rostock, Germany — [2]Radboud University Nijmegen, Institute for Molecules and Materials, 6525 AJ Nijmegen, The Netherlands

Long-lived excitons are a promising pathway for energy transfer over long distances. Here we show that self-organized porphyrin nanostructures host excited states with surprisingly long lifetimes. The molecule aggregates are investigated by spatially and time-resolved photoemission electron microscopy (PEEM). While time-resolved fluorescence spectroscopy reveals lifetimes in the nanosecond range, additional decay processes are observed by PEEM with substantially longer time constants. These optically dark states may enable an efficient energy transport channel within the aggregates.

O 47.5 Tue 18:15 Poster E

Towards ToF Momentum Microscopy With CW Sources Using an Ultrafast Chopper Scheme — •Anna Zaporozhchenko[1,2], Olena Fedchenko[1], Katerina Medjanik[3,1], Sergej Chernov[1], Andreas Oelsner[4], Hans-Joachim Elmers[1,2], and Gerd Schönhense[1,2] — [1]Institut für Physik, JOGU, 55099 Mainz, Germany — [2]Graduate School of Excellence MAINZ, 55128 Mainz, Germany — [3]Lund University, MAX IV Laboratory, 22100 Lund, Sweden — [4]Surface Concept GmbH, 55124 Mainz, Germany

The use of time-of-flight techniques for high-resolution spectroscopy and momentum microscopy requires a defined time structure of the photon beam. The time resolution of 3D (x,y,t)-resolving detectors, e.g. the delay-line detector, is typically 150 ps [1]. Thus a period of the exciting photon pulses of 200 ns (pulse rate of 5 MHz) yields more than 1000 time slices, sufficient for high-resolution spectroscopy. We developed an ultrafast electron-optical deflector system capable of chopping the desired pulse repetition rate out of a faster pulse train or even out of a continuous-wave signal. A first experiment with a laboratory He source was performed. In the first prototype pulse profiles of 2 ns width have been achieved. One goal is to chop lower pulse rates from the 100 or 500 MHz multibunch signal of storage rings. The current status of this development will be shown. Funded by BMBF (05K13UM1)

O 47.6 Tue 18:15 Poster E

Investigation of Coronene Thin-Films on Ag(111) Using Photoelectron Spectroscopy — •Christian Udhardt, Felix Otto, Tino Kirchhübel, Falko Sojka, Tobias Hümpfner, Bernd Schröter, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Several metal-intercalated aromatic hydrocarbons, including potassium intercalated coronene, were found to have superconductive properties [Kubozono et. al, Phys. Chem. Chem. Phys. **13**, 16476 (2011)]. Preparing and investigating the organic materials as thin films on various substrates can give access to the underlying mechanisms of the observed superconductivity and make the materials available for a potential use in electronic devices. Here we characterized the electronic structure of the coronene molecules prepared as thin films in the monolayer range on Ag(111) using ultraviolet and X-ray photoelectron spectroscopy (UPS and XPS). Comparing the results of k_x, k_y -dependent UPS measurements with those from low-energy electron diffraction (LEED) and density functional theory (DFT) calculations we were able to reconstruct the alignment of the coronene molecules with respect to the Ag(111) surface. Results after doping the films with potassium are presented as well.

O 47.7 Tue 18:15 Poster E

Low temperature scanning tunneling microscopy investigation of the phase change material $Ge_2Sb_2Te_5$ — •Daniel Montag[1], Jens Kellner[1], Christian Pauly[1], Marcus Liebmann[1], Alessandro Giussani[2], Volker Deringer[3], Raffaella Calarco[2], Richard Dronskowski[3], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University, Germany — [2]Paul Drude Institut für Festkörperelektronik, Berlin, Germany — [3]Institute of Inorganic Chemistry, RWTH Aachen University, Germany

We present a scanning tunneling microscopy (STM) study of the phase change material $Ge_2Sb_2Te_5$ (GST), epitaxially grown on Si(111) in the metastable cubic phase and transferred in-situ in ultrahigh vacuum from the molecular beam epitaxy system to the STM. Despite the fact that GST is already commercially used, there is still no complete understanding of the ultra fast switching speed, the strong resistance change, and the high endurance of the Ge-Sb-Te alloys. One contribution to such a theory is an atomic scale understanding of the electronic properties of GST including the disorder caused by the relatively high vacancy content in the GeSb layers. We present $\frac{dI}{dV}$-field measurement on the atomic scale conducted at 8K. The analysis shows spatial fluctuations of the valence band onset and the gap width, wich is probably related to a random distribution of the Ge and Sb atoms. Moreover, particular structures within the STM images probing mainly the surface Te layer are compared with density functional theory calculations.

O 47.8 Tue 18:15 Poster E

Fermi surface mapping of the phase change material $Ge_2Sb_2Te_5$ by photoelectron spectroscopy — •Jens Kellner[1], Marcus Liebmann[1], Christian Pauly[1], Jos Boschker[2], Rui Ning Wang[2], Evangelos Golias[3], Jaime Sanchez-Barriga[3], Oliver Rader[3], Raffaella Calarco[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen — [2]Paul Drude Institut für Festkörpelektronik, Berlin — [3]Helmholtz-Zentrum, BESSY, Berlin

Phase change materials (PCM) have become essential components of optical memories (DVD-RW, Blu-ray Disc, ...) and they are important candidates for future non-volatile computer memories. Understanding the fundamental electronic properties would thus be important to improve the phase change characteristics. We present an angle-resolved photoemission (ARPES) study of the ternary PCM $Ge_2Sb_2Te_5$, epitaxially grown on Si(111) in the metastable cubic phase. The sample was transferred in-situ in ultrahigh vacuum from the molecular beam epitaxy system to the analysis chamber, where we performed a three-dimensional mapping of the band structure by variation of the photon energy (15-31 eV). The states close to the Fermi energy, which are contributing to the transport, are used to construct three-dimensional constant energy surfaces mimicking the Fermi surface relevant for the metallic conductivity of the crystalline phase. Additional spin-polarized ARPES measurements identify a surface state close to the Fermi level with a spin polarization of nearly 100%.

O 47.9 Tue 18:15 Poster E

Investigation of the Potassium-Doping of Tetraphenyldibenzoperiflanthene (DBP) on Ag(111) by Photoelectron Spectroscopy — •Felix Otto, Christian Udhardt, Tino Kirchhuebel, Bernd Schroeter, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Tetraphenyldibenzoperiflanthene (DBP, $C_{64}H_{36}$) has been explored for some years because of its possible use in organic electronics [1]. DBP consists of an aromatic backbone with four phenyl rings attached nearly perpendicular to the molecular plane. We analysed the change of electronic properties due to the doping process of this organic dye with potassium. Special attention is paid to the possible adsorption sites of the potassium atoms in the organic/inorganic heterosystem. We used *in situ* differential reflectance spectroscopy (DRS) to determine changes of the optical properties due to the potassium deposition [2, 3]. These results are compared with x-ray (XPS) and ultraviolet photoelectron spectroscopic (UPS) measurements to elucidate the charge transfer between the alkali metal and DBP. Furthermore effects on the electronic structure are discussed in terms of lowest unoccupied molecular orbital (LUMO) filling and the evolution of an interface dipole.

[1] J. D. Debad *et al.*, J. Am. Chem. Soc. **118**, 2374 (1996).

[2] R. Forker and T. Fritz, Phys. Chem. Chem. Phys. **11**, 2142 (2009).

[3] R. Forker *et al.*, Annu. Rep. Prog. Chem., Sect. C: Phys. Chem. **108**, 34 (2012).

O 47.10 Tue 18:15 Poster E

Thickness dependent electronic structure and Kondo resonance of $CePt_5$ on Pt(111) — •Katharina Treiber, Henriette Maass, Holger Schwab, Hendrik Bentmann, and Friedrich Reinert — Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg

At low temperatures local interactions between Ce *4f*— and conduction electrons in thin films of $CePt_5$ on Pt(111) lead to a spectral feature at the Fermi surface — the Kondo resonance [1]. At even lower temperatures heavy quasiparticles interact and form coherent heavy fermion bands at the Fermi-level [2]. Whereas previous studies showed that the $CePt_5$ surface alloy appears in a variety of different phases depending on Ce coverage and post annealing procedure [3], most photoemission studies have been carried out on a phase occurring at a surface coverage of four unit cells $CePt_5$ on Pt(111).

In this contribution we examine the electronic structure of the different surface phases by angle-resolved photoemission (ARPES) at low temperatures considering Fermi surface, Kondo resonance and bandstructure. Furthermore, we explore the Kondo temperature which recently has been suggested to show a dependency on the $CePt_5$ film thickness on the basis of x-ray absorption spectroscopy and x-ray magnetic circular dichroism studies [4].

[1] M. Garnier *et al.*, Phys. Rev. B **56**, R11399(R), (1997)

[2] M. Klein *et al.*, Phys. Rev. Lett. **106**, 186407, (2011)

[3] J. Tang *et al.*, Phys. Rev. B **15**, 15342, (1993)

[4] C. Praetorius *et al.*, Phys. Rev. B **92**, 045116, (2015)

O 47.11 Tue 18:15 Poster E

Spin-orbit interaction in Pb monolayers on Si(111) — •Christian Brand[1], Haiyue Liu[1], Philipp Kröger[1], Herbert Pfnür[1], Gabriel Landolt[2,3], Jan-Hugo Dil[2,4], Stefan Muff[2,4], Michael C. Tringides[5], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Germany — [2]Swiss Light Source, Villigen, Switzerland — [3]Universität Zürich, Switzerland — [4]École Polytechnique Fédérale de Lausanne, Switzerland — [5]Ames Laboratory & Iowa State University, Ames, USA

Atomic monolayers (ML) of Pb/Si(111) have recently been found to be superconducting below $T_C \approx 1.6\,K$, but the mechanism behind the evolution of these 2d states is yet not understood. In the range from $6/5\,ML$ to $4/3\,ML$ supercells consisting of linear combinations of $\sqrt{7} \times \sqrt{3}$ and $\sqrt{3} \times \sqrt{3}$ unit cells are formed (so-called Devil's staircase regime). This allows us to the tune spin-orbit interaction (SOI), the electronic and atomic structure via adsorption of minute amounts of Pb. In this study we present (SR)-ARPES, DC-, and magneto-transport measurements at low T ($> T_C$) to evaluate the influence of SOI on the Pb surface states. As derived from magneto-transport weak-antilocaization occurs indicating strong SOI, while Hall resistance slopes shows pure n-type conductivity. The carrier concentrations agree well with EDCs from ARPES, while SR-MDCs reveal a complex spin-texture at E_F in Pb surface states around the surface high symmetry points. Moreover, Pb induced high Schottky barriers at highly n-doped substrates reveal new insights into hybridization of Si bulk states in valence band by confinement effects near the surface.

O 47.12 Tue 18:15 Poster E

Scanning Tunneling Microscopy study of a newly proposed Topological Insulator $ZrTe_5$ — •Timo Kuhn[1], Luca Gragnaniello[1], Gabriel Autès[2], Giulia Manzoni[4], Alberto Crepaldi[3], Fulvio Parmigiani[3], Helmuth Berger[2], Oleg Yazyev[2], and Mikhail Fonin[1] — [1]Universität Konstanz, Universitätsstraße 10, 78464 Konstanz, Germany — [2]Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [3]Elettra-Sincrotrone Trieste, Strada Statale 14, 34149 Basovizza, Trieste, Italy — [4]Universitá degli Studi di Trieste, Via A. Valerio 2, Trieste 34127, Italy

Topological insulators belong to a new kind of material class that posses robust gapless states inside the insulating bulk gap, which makes them promising candidates for achieving dissipationless transport devices. We present a Scanning tunneling microscopy (STM) and spectroscopy (STS) study on a layered material $ZrTe_5$, a promising candidate for a new topological insulator. The crystal structure could clearly be identified in topography images. STM measurements enabled direct imaging of standing waves at steps and defects. The standing waves show a clearly dispersive character. Furthermore STS measurements are in good agreement with density functional theory calculations and reveal Landau quantization with applied magnetic field. Comparison with data obtained by angle resolved photoemission spectroscopy allows for detailed insights into the electronic properties of this material.

O 47.13 Tue 18:15 Poster E

Probing the electronic structure of epitaxially grown topological insulators with varying magnetic doping — •Sonja Schatz[1], Mohammed Al-Baidhani[1], Thiago R. F. Peixoto[1], Henriette Maass[1], Christoph Seibel[1], Hendrik Bentmann[1], Grzegorz Karczewski[2,3], Steffen Schreyeck[2], Martin Winnerlein[2], Charles Gould[2], Karl Brunner[2], Laurens Molenkamp[2], and Friedrich Reinert[1] — [1]Experimentelle Physik

VII, Universität Würzburg, D-97074 Würzburg — [2]Experimentelle Physik III, Universität Würzburg, D-97074 Würzburg — [3]Institute of Physics, Polish Academy of Science, 02-668 Warsaw, Poland

We will present an overview of recent photoelectron spectroscopy (PES) studies of epitaxial topological insulator (TI) thin films. In particular, we investigated (BiSb)$_2$Te$_3$ layers with a particular focus on magnetic doping with V and Cr impurities. X-ray photoemission (XPS) and absorption measurements of the $2p$ core level lines provide information on the incorporation of the impurities in the TI host material. Resonant PES allows us to address the V $3d$ states in the valence band which are expected to play a crucial role for the exotic magnetic and transport properties of these systems. Furthermore, angle-resolved PES of the topological surface state in Bi$_2$Se$_2$Te films will be presented, focusing on anisotropy effects in the Fermi surface [1]. The strength of the anisotropy lies between Bi$_2$Se$_3$ and Bi$_2$Te$_3$. Angle-dependent XPS is used to characterize chemical shifts in the core level lines and to obtain information of the chemical composition near the surface [1].

[1] H. Maaß *et al.*, J. Appl. Phys. **116**, 193708, (2014)

O 47.14 Tue 18:15 Poster E

Alpha-Sn: doping and Te coating study — •Caroline von Andrian-Werburg, Markus Scholz, Felix Reis, Victor Rogalev, Ralph Claessen, and Jörg Schäfer — Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

Topological insulators (TIs) promise an outstanding progress in transformation of conventional electronics to spintronics. In that scope mono-elemental 3D TIs would have a significant advantage due to the simplicity of growth and defect control. However, the only example described so far is the low temperature phase of Sn (α-Sn) [1]. Recently it was found that using Molecular Beam Epitaxy one can stabilize the low-T phase of Sn with topological character on a substrate with a slightly mismatched lattice (0, 14%)[2]. This compressive strain induces a gap at the Fermi level of the otherwise gapless α-Sn with band inversion, thus enabling the occurrence of the topological surface states. In the current study we explore further important steps towards the technological application of α-Sn, namely, the possibility of doping to vary the position of the Fermi level and protective capping of the film. The protective layer is required in case of ex-situ transfer operations. For both purposes we find elemental Te to be a suitable candidate. A small amount of the Te during the co-deposition with Sn allows to introduce a n-doping of the material, while the amorphous Te overlayer protects the surface from the unnecessary contamination and can be removed by moderate annealing.

[1] L. Fu and C. L. Kane, Phys. Rev. B. 76, 045302 (2007).
[2] A. Barfuss et al., Phys. Rev. Lett. 111, 157205 (2013).

O 48: Electronic Structure: Surface Magnetism and Spin Phenomena

Time: Tuesday 18:15–20:30 Location: Poster E

O 48.1 Tue 18:15 Poster E

High-Mobility Sm-Doped Bi2Se3 Ferromagnetic Topological Insulators and Robust Exchange Coupling — •Taishi Chen — Max Plank Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Magnetically doped topological insulators (MTIs) are emerging as a new platform of dilute magnetic semiconductors (DMSs) as a result of growing interest in topological magnetoelectric effect, the quantum spin/anomalous Hall Effect, and Dirac fermion-mediated magnetic coupling physics [1]. However, the traditional transition metal magnetic elements doped topological insulators are often hindered by the inadequate material quality, which is demonstrated by the low mobility of the samples [2-4]. In this work [5], we show the successful preparation of a series of new Sm-doped Bi2Se3 MTIs, which exhibit ferromagnetism up to about 52 K and a suppressed bulk electron carrier concentration as low as 1018 cm*3 in order. Clear Shubnikov*de Haas oscillations are observed in these samples. All evidence suggests that Sm-doped Bi2Se3 is a candidate high-mobility MTI.

O 48.2 Tue 18:15 Poster E

High-Mobility Sm-Doped Bi2Se3 Ferromagnetic Topological Insulators and Robust Exchange Coupling — •Taishi Chen — Max Plank Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Magnetically doped topological insulators (MTIs) are emerging as a new platform of dilute magnetic semiconductors (DMSs) as a result of growing interest in topological magnetoelectric effect, the quantum spin/anomalous Hall Effect, and Dirac fermion-mediated magnetic coupling physics [1]. However, the traditional transition metal magnetic elements doped topological insulators are often hindered by the inadequate material quality, which is demonstrated by the low mobility of the samples [2-4]. In this work [5], we show the successful preparation of a series of new Sm-doped Bi2Se3 MTIs, which exhibit ferromagnetism up to about 52 K and a suppressed bulk electron carrier concentration as low as 1018 cm*3 in order. Clear Shubnikov*de Haas oscillations are observed in these samples. All evidence suggests that Sm-doped Bi2Se3 is a candidate high-mobility MTI.

References [1] X. L. Qi, et al., Physical Review B 78, 195424 (2008). [2] C. Z. Chang, et al., Science 340, 6129, (2013). [3] C. Z. Chang, et al., Nature Materials 14, 5, (2015). [4] Y. L. Chen, et al., Science 329, 5992, (2010). [5] T. S. Chen, et al., Advanced Materials 27, 33, (2015).

O 48.3 Tue 18:15 Poster E

Laser induced DC photocurrents in a Topological Insulator thin film — •Nina Meyer[1], Thomas Schumann[1], Dagmar Butkovicová[2], Eva Schmoranzerová[2], Helena Reichlová[3], Gregor Mussler[4], Petr Nemec[2], Detlev Grützmacher[4], and Markus Münzenberg[1] — [1]Institute of Physics, Ernst-Moritz-Arndt University, Greifswald,Germany — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [3]Institute of Physics ASCR v.v.i., Prague, Czech Republic — [4]Peter Grünberg Institute (PGI-9), Jülich, Germany

Recent experiments give evidence that the optical excitation of spin-polarized surface states of topological insulators (TI) can launch electron currents along the surface whose direction can be controlled by varying the polarization of the driving light [1]. We generated a photocurrent by illuminating TI (Bi, Sb)$_2$Te$_3$ thin films with laser light whose polarization changes periodically. The laser light was focused to a 6 μm spot on the device by an objective. We found and will discuss that the photocurrent has at least two parts on different time dynamics. Furthermore we determined different Parameters like [1] and show their dependence on polarization and additional experimental parameters. The films with a thickness of 20 nm were structured to Hall bar devices.

We acknowledge funding through DFG priority program SPP "Topological Insulators" and DAAD PPP Czech Republic "FemtomagTopo".
[1] J. W. McIver, D. Hsieh, H. Steinberg, P. Jarillo-Herrero and N. Gedik, Nature Nanotechnology 7, 96-100 (2012)

O 48.4 Tue 18:15 Poster E

W(110) and Ta(110): A Playground for Spin-Orbit-Induced Effects on Surface States — •H. Wortelen[1], K. Miyamoto[2], H. Mirhosseini[3], B. Engelkamp[1], A.B. Schmidt[1], J. Henk[4], and M. Donath[1] — [1]Universität Münster — [2]HSRC, Hiroshima University — [3]MPI für Mikrostrukturphysik Halle — [4]Universität Halle-Wittenberg

The influence of spin-orbit effects on the surface electronic structure of W(110) and Ta(110) was investigated with spin- and angle-resolved photoemission and inverse photoemission experiments and electronic-structure calculations. We present a comprehensive $E(\mathbf{k}_\parallel)$ picture of the electronic states and their spin texture in the occupied and unoccupied regime.

Tungsten and tantalum, direct neighbors in the periodic table, exhibit a very similar electronic structure, yet with a shifted Fermi energy due to the one electron difference. Both elements exhibit a bcc crystal structure, however, with different lattice parameters resulting in differently pronounced hybridization of surface and bulk bands. As a consequence, a Dirac-cone-like surface state, reminiscent of a topological surface state, observed for W(110) below E_F [1,2] has no apparent equivalent on Ta(110), although it is expected above E_F [3]. Furthermore, a Rashba-split d_{z^2} surface state appears on Ta(110) [4], which has no equivalent on W(110).

[1] Miyamoto et al., Phys. Rev. Lett. **108**, 066808 (2012)

[2] Mirhosseini et al., New J. Phys. **15**, 033019 (2013)
[3] Engelkamp et al., Phys. Rev. B **92**, 085401 (2015)
[4] Wortelen et al., Phys. Rev. B **92**, 161408(R) (2015)

O 48.5 Tue 18:15 Poster E

First-principles dynamical spin and charge currents in magnetic nanostructures — •Sascha Brinker, Filipe Souza Mendes Guimarães, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We investigate the spatial distribution of ground state and dynamical spin and charge currents in magnetic nanostructures from first-principles. We outline our density functional theory implementation in the Korringa-Kohn-Rostoker Green function method, in a real-space approach. Small magnetic nanostructures are considered, e.g. Fe adatoms, dimers and trimers on the Au(111) and Pt(111) surfaces. Our findings should be relevant for recent and future microscopy techniques [1].

Work funded by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] A. Lubk, A. Béché, and J. Verbeeck, Phys. Rev. Lett. **115**, 176101 (2015)

O 48.6 Tue 18:15 Poster E

Bi/Ag(111) vs. Pb/Ag(111) along $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{K}}$ – A comparative study of the unoccupied states — •Katharina T. Ritter[1], Sune N. P. Wissing[1], Anke B. Schmidt[1], Hossein Mirhosseini[2], Steven Achilles[3], Jürgen Henk[3], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany

Surface alloys of heavy metal elements on noble metal surfaces exhibit strongly Rashba-split band structures. Especially surface alloys with $(\sqrt{3}\times\sqrt{3})R30^\circ$ reconstruction have been investigated over the last few years.

Here, we compare Bi/Ag(111) and Pb/Ag(111) systematically. We present spin- and angle-resolved inverse photoemission data for both high-symmetry directions $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{K}}$. The experimental data is complemented by theoretical calculations.

Changing the adsorbate from Bi to Pb results in an energetic shift of the surface states and leads to a different size of the spin splitting. These changes are attributed to the adsorbate's atomic number, which is connected to the atomic spin-orbit coupling, as well as to its size, thus the relaxation of the surface.

O 48.7 Tue 18:15 Poster E

Spin filtering in Bi superstructures on a Au(111) surface — Sebastian Jakobs[1,2], •Dominik Jungkenn[1], Christian Tusche[3], Jürgen Kirschner[3], Benjamin Stadtmüller[1], Mirko Cinchetti[1], Stefan Mathias[4], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str 46, 67663 Kaiserslautern, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany — [3]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 062120 Halle/Saale, Germany — [4]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Spin dependent scattering of electrons at interfaces is one of the most relevant microscopic processes that determine the performance of spintronics devices. However, the scattering process itself is hard to address experimentally. Here, we use spin-resolved momentum microscopy to investigate the scattering of photoelectrons from a Au(111) surface on Bi superstructures. We will show that the Bi/Au(111) interface constitutes a simple model system to understand spin dependent electron scattering processes on the microscopic level, since the spin polarization changes with the number and direction of scattering events.

O 48.8 Tue 18:15 Poster E

Inelastic spin excitations and many-body effects in Fe porphins — •Laëtitia Farinacci, Nino Hatter, Sonja Schubert, Benjamin W. Heinrich, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Magnetism of 3d metals in molecules is commonly treated by crystal field theory. Nonetheless, in case of strong hybridization of the d levels with ligand orbitals this approach may be insufficient. Modification of the conjugated π system could give insight in the influence of such hybridization effects.

Using STM and STS we investigate the properties of the H2P porphins adsorbed on Au(111). After deposition, only monomers are observed on the surface. Annealing to 630 K triggers their polymerization and metalation of the molecules is achieved by Fe deposition at 300 K.

In spectroscopy, FeP monomers and dimers present various features around the Fermi energy above their Fe centers as well as above specific parts of their molecular ligand. Depending on the nature and adsorption site of the molecules, steps localized at energies up to ± 14 mV as well as a zero bias anomaly similar to a Fano-line shape can be observed. These features result from an interplay between inelastic spin excitations and many-body effects: their shape, broadening and localization cannot be fully addressed by crystal field theory and have to be related to the mixing of the Fe d levels with organic orbitals reported by theory [1] as well as to various couplings to the substrate.

[1] M.E. Ali, et al., J. Phys. Chem. B 116, 5849 (2012).

O 48.9 Tue 18:15 Poster E

Correlation effects in the surface electronic structure of Fe(110) — •Beatrice Andres, Marko Wietstruk, and Martin Weinelt — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Beyond one-electron mean-field theories, electronic band energies are renormalized by many-body effects. Such a renormalization can directly be observed in photoemission as a kink in the band dispersion, where the band reaches the excitation energy of a quasi particle. In laser photoemission ($h\nu = 6.2$ eV) on Fe/W(110) we find an occupied surface band crossing the Fermi level at ~ 0.1 Å^{-1} in Γ-H direction. We observe a pronounced energy renormalization in this iron minority-spin surface state at 160 meV binding energy. Following Ref. [1], we assign this to a renormalization by magnon dressing of the surface electrons.

Applying spin-resolved photoemission, we are able to track the spin polarization of the surface band and ensure that the observed kink is not a trivial crossing of two bands. Our spin detection is based on exchange scattering at a magnetized Fe/W(001) target. By switching the magnetization of sample and scattering target separately, we are able to distinguish between spin polarization and dichroic effects in the photoemission process. Thereby, we find the magnetic-linear-dichroic contrast changing sign crossing the kink as expected for spin-momentum coupling.

[1] Jörg Schäfer, *Phys. Rev. Lett.* **92**, 097205 (2004)

O 48.10 Tue 18:15 Poster E

Non-collinear spin-states in dilute 1D chains induced by Dzyaloshinskii-Moriya interaction — •Manuel Steinbrecher[1], Alexander Ako Khajetoorians[1,2], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]INF, Hamburg University, 20355 Hamburg, Germany — [2]IMM, Radboud University, 6525 AJ Nijmegen, The Netherlands

Nanostructures of coupled atomic spins are of high interest for future spintronic applications. Therefore, a deep understanding of the behavior of single magnetic atoms deposited on metallic surfaces and of the coupling between several of these spins is mandatory. By using the tip of a scanning tunneling microscope as a tool, single atoms can be moved on a surface [1] to build artificial nanostructures. Realizing bottom-up fabricated 1D spin chains so far led to simple ferromagnetic [2] or antiferromagnetic [3] ground states described by Néel states [4,5]. When using a heavy spin-orbit coupling material, like a Pt(111) surface [6], as a substrate we showed that we can tune the strength of an anisotropic, indirect exchange interaction between indidivual Fe atoms, namely the Dzyaloshinskii-Moriya interaction [7]. With this knowledge we were able to build 1D spin chains and induce non-collinear spin states in the chains, resulting in exotic magnetic behavior. [1] Eigler and Schweizer, Nature **344**, 524 (1990); [2] Gambardella *et al.*, Nature **416**, 301 (2002); [3] Hirjibehedin *et al.*, Science **312**, 1021 (2006); [4] Khajetoorians *et al.*, Science **332**, 1062 (2011); [5] Khajetoorians *et al.*, Nat. Phys. **8**, 497 (2012); [6] Khajetoorians *et al.*, PRL **111**, 157204 (2013); [7] Khajetoorians *et al.*, Nat. Commun., submitted (2015)

O 49: Metal Substrates: Structure, Adsorption and Growth

Time: Tuesday 18:15–20:30 Location: Poster E

O 49.1 Tue 18:15 Poster E

On the microscopic structure of the Ag(441) surface — •Thorsten Wagner, Robert Zimmerleiter, Daniel Roman Fritz, and Peter Zeppenfeld — Johannes Kepler University Linz, Institute for Experimental Physics, Austria

Regularly stepped (vicinal) surfaces provide a convenient path to control the number of defects of a surface. They can be easily prepared by a slight miscut of a low index surface. In the case of an fcc(nn1) surface with small integer n it is even expected that the large number of steps will dominate the surface properties. Here we report on a study of the Ag(441) surface using a combination of scanning tunneling microscopy (STM) and high resolution electron diffraction (SPA-LEED). The STM data suggest a statistical distribution of the step width which can be described by a Γ-probability distribution. In fact, the steps are not randomly distributed but are interacting. The detailed statistical analysis of the images also reveals that the terraces are formed by an integer number of (331) building blocks whereas the actual steps are given by (551) microfacets. In order to compare the electron diffraction data to the real space information from the STM experiment, we carried out simulations of the reciprocal space maps (RSM) in the framework of the simple kinematic approximation. In the case of narrow, interacting steps one has to be cautious to carry out a correct interpretation of the experimental RSM based on the splitting of the rods and their tilt angle, only. Especially the latter is strongly influenced by the correct alignment of the sample.

O 49.2 Tue 18:15 Poster E

DFT-based survey of site dependent interaction of halogen atoms with the (001) surfaces of Cu, Ag, and Au — •Alexandra C. Dávila, Lukas Deuchler, Sönke Buttenschön, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

Diffusion at electrochemical interfaces is a decisive factor for, e.g., metal electrodeposition using halogen ion containing electrolytes [1]. The potential dependent growth has been ascribed to the variation of activation energy barriers due to the interaction of adsorbate-induced electric dipoles with the electric field at the surface [1,2]. In order to identify trends that may be relevant for the diffusion of halogen atoms on coinage metal (001) surfaces, we present a survey based on density functional total energy calculations with VASP [3,4] for the potential energy surface calculated for particular geometries corresponding to halogen atoms at the hollow, bridge, and top sites, and the associated electric dipole moments. Results both for separated halogen atoms and for coverage $\Theta = 0.5$ are compared to DFT data from the literature, e.g. Ref. [5].

[1] M. Ruge, F. Golks, J. Zegenhagen, O.M. Magnussen, J. Stettner, Phys. Rev. Lett. **112**, 055503 (2014).

[2] M. Giesen, G. Beltramo, S. Dieluweit J. Müller, H. Ibach, W. Schmickler, Surf. Sci. **595**, 127 (2005).

[3] G. Kresse, J. Hafner, Phys. Rev. B **49**, 14251 (1994).

[4] //www.vasp.at.

[5] A. Migani, F. Illas, J. Phys. Chem B **110**, 11894 (2006).

O 49.3 Tue 18:15 Poster E

Diffusion properties of lithium studied using DFT: growth phenomena and the effect of an electric field — •Markus Jäckle[1,2] and Axel Gross[1,2] — [1]Helmholtz Institut Ulm - Elektrochemische Energiespeicherung, 89069 Ulm, Germany — [2]Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The formation of dendrites poses a big problem in batteries and can lead to short-circuits during battery operation. As metal growth processes are intimately linked to diffusion, we have extended our initial theoretical first-principles study of the self-diffusion properties of lithium [1], in order to enhance our understanding of a possible explanation for this phenomenon which may help avoiding battery failure due to dendrite growth.

According to our calculations, the previously established picture of an inhomogeneous lithium surface [1] is correct. The new results further suggest that the (011) surface of lithium may have an important role in facilitating the growth of dendrites and that the effect of an electric field on lithium self-diffusion is rather small.

[1] M. Jäckle and A. Groß, J. Chem. Phys. **141**, 174710 (2014).

O 49.4 Tue 18:15 Poster E

Growth and potassium doping of ultrathin layers of picene on Ag(100) — •Martin Hafermann[1], Tobias Huempfner[1], Roman Forker[1], and Torsten Fritz[1,2] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Osaka University, Graduate School of Science and Institute for Academic Initiatives, Department of Chemistry, 1-1 Machikaneyama, Toyonaka 560-0043, Osaka, Japan

Superconductivity in polycyclic aromatic hydrocarbons (PAH) was discovered in alkali-metal-intercalated solid picene [1]. A more recent study questions the very superconductivity in K_3picene and calls for more accurate structural characterizations of such systems, especially of their low-dimensional structures [2]. In this contribution we investigate ultrathin films of potassium-doped picene on Ag(100) to obtain a deeper understanding of the mechanisms causing the superconductive properties of PAHs. To analyze the growth of the pristine picene layers as well as the potassium-doping process we used scanning tunneling microscopy (STM) and distortion-corrected low-energy electron diffraction (LEED). We determined that the epitaxy of the picene monolayer on Ag(100) exhibits a point-on-line coincidence, and that the lattice parameters correspond to a bulk-like unit cell consisting of two molecules, one flat lying and one tilted with respect to the substrate surface. Potassium intercalation into one monolayer picene on Ag(100) led to the formation of a new commensurate phase.

[1] R. Mitsuhashi *et al.*, Nature **464**, 76 (2010).

[2] S. Heguri *et al.*, Phys. Rev. B **92**, 014502 (2015).

O 49.5 Tue 18:15 Poster E

Thin epitaxial films of tetraphenyldibenzoperiflanthene (DBP) on Ag(111) — •Tino Kirchhuebel[1], Marco Gruenewald[1], Falko Sojka[1], Satoshi Kera[2,3,4], Fabio Bussolotti[2], Takahiro Ueba[2,3], Nobuo Ueno[4], Gaël Rouillé[5], Roman Forker[1], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany — [2]Institute of Molecular Science, Myodaiji, Okazaki, Japan — [3]SOKENDAI, The Graduate University of Advanced Studies, Okazaki, Japan — [4]Graduate School of Advanced Integration Science, Chiba University, Japan — [5]Institute of Solid State Physics & Laboratory Astrophysics Group of the Max Planck Institute for Astronomy, Friedrich Schiller University Jena, Germany

We investigated epitaxial tetraphenyldibenzoperiflanthene (DBP) thin films grown on Ag(111). Structural characterization using LEED and STM revealed a well-ordered flat-lying thin film grown in a herringbone arrangement within the first monolayer. In order to trace the development of the optical properties *in situ* differential reflectance spectroscopy (DRS) was performed. A strong interaction between molecules in contact with the Ag(111) surface was found. Depending on the coverage two distinct spectral fingerprints of DBP molecules on top of the first monolayer arise, indicating a transformation from DBP monomers to aggregates. Ultraviolet photoelectron spectroscopy (UPS) measurements reveal two distinct sets of peaks for the occupied states of DBP multilayer samples on Ag(111), being indicative of an individual alignment of electronic states for each DBP species.

O 49.6 Tue 18:15 Poster E

A Giant Molecular Spoked Wheel — •Stefan-Sven Jester, Robert May, and Sigurd Höger — Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn

The modular synthesis of a defined, rigid molecular spoked wheel structure with the sum formula $C_{1878}H_{2682}$ and a diameter of about 12 nm is described. The attached 96 dodecyl side chains provide the solubility of the 25260 Da compound in common organic solvents. At the octanoic acid/highly oriented pyrolytic graphite interface, the molecules self-assemble to form an ordered 2D lattice, which is investigated by scanning tunneling microscopy, displaying their structure with submolecular resolution. [1] R. May, S.-S. Jester, S. Höger *J. Am. Chem. Soc.* **2014**, *136*, 16732-16735.

O 49.7 Tue 18:15 Poster E

Nanopatterning by rod-bridge-rod-shaped molecules — •Stefan-Sven Jester, Melissa Hündgen, Katharina Anna Weis, and Sigurd Höger — Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn

The supramolecular self-assembly of arylene-alkynylenes with a rod-bridge-rod geometry is investigated at the solution/solid interface. Scanning tunneling microscopy provides a submolecularly resolved insight into the 2D nanostructures that are formed on the graphite surface, which acts as a template. We focus on how the nanopatterns depend on their molecular building blocks. In particular, we investigate how shape and shape-persistence of the backbones, their alkyl/alkoxy side-chain periphery and the rod end groups influence the pattern structures.

O 49.8 Tue 18:15 Poster E

Structure and electronic properties of triazatruxene layers on Ag(111) studied by LT-STM — •Anja Bauer[1], Florian Singer[1], Philipp Erler[1], Markus Maier[2], Rainer Winter[2], Luca Gragnaniello[1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Fachbereich Chemie, Universität Konstanz, Konstanz, Germany

We present a study of triazatruxene (TAT) molecules deposited on Ag(111) by means of electrospray ionization in ultra high vacuum. We investigated the structural and electronic properties of TAT molecules at different coverages by means of low temperature scanning tunneling microscopy (STM) and spectroscopy (STS). For coverages far below one monolayer we observe the molecular superstructures which are stabilized by long-range repulsive intermolecular interaction. High-resolution STM imaging reveals three different types of intramolecular structure, which are possibly due to different site-specific interaction between the molecule and the substrate. At coverages close to one monolayer we observe the formation of self-assembled structures. Here, three different packing types are observed. Depending on the exact surrounding of each molecule within the layer a strong variation in the orbital structure of the molecules is observed. We attribute this findings to a strong surface-enhanced dipol-dipol interaction between the molecules.

O 49.9 Tue 18:15 Poster E

Adsorbate nanomesh causes lateral segregation: Ab-initio based Monte–Carlo study for *h*-BN on Pt$_{50}$Rh$_{50}$(111) — •Wolfgang Heckel[1], Tobias C Kerscher[1], Roland Stania[2,3], Thomas Greber[2], and Stefan Müller[1] — [1]Hamburg University of Technology, Institute of Advanced Ceramics — [2]Universität Zürich, Physik-Institut — [3]Paul Scherrer Institut Villigen, Swiss Light Source

Surface segregation in metal alloys and its adjustability by adsorbates is a well-known phenomenon [1]. In our study, Pt–Rh serves as a substrate for a self-assembled 2d boron nitride (*h*-BN) layer. The experiments on *h*-BN/Pt$_{50}$Rh$_{50}$(111) show a corrugated, honeycombed 11×11 nanomesh adsorbate layer caused by the lattice constant mismatch of substrate and adsorbate [2].

Using a combined DFT–cluster-expansion approach we elucidate the laterally periodic segregation profile of PtRh(111) caused by *h*-BN. Our results perfectly confirm the experiment: Beneath pores of the nanomesh the segregation profile shows a strong Rh enrichment, while beneath wires the topmost layer favors platinum.

To quantify the Pt/Rh content per surface layer, we conducted Monte–Carlo simulations accomodating the chemical potential difference of the alloy constituents and the quenched Pt/Rh interdiffusion at low temperatures. In agreement with the experiment, we find that a further Pt enrichment in the top surface layers is favored at elevated temperatures.

[1] Kerscher et al., Phys. Rev. B **86**, 195420 (2012)

[2] Stania et al., submitted.

O 49.10 Tue 18:15 Poster E

Vacuum Synthesis of Magnetic Aluminum Phthalocyanine on Au(111) — Chao Li and •Yongfeng Wang — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China.

Air-unstable magnetic aluminum phthalocyanine (AlPc) molecules are prepared by an on-surface metalation reaction of phthalocyanine with aluminum (Al) atoms on Au(111) in ultrahigh vacuum. STM/STS experiments and DFT calculations show that an unpaired spin is located on the conjugated isoindole lobes of the molecule rather than at the Al position. These results demonstrate the success of the vacuum synthesis of an air-unstable magnetic molecule. It is interesting and important to synthesize other pristine reactive MPc molecules and study their particular properties.

O 49.11 Tue 18:15 Poster E

A first-principles study of chemo-mechanical coupling for hydrogen on Ir(111) — •Anja Michl, Gregor Feldbauer, and Stefan Müller — Hamburg University of Technology, Institute of Advanced Ceramics

Mechanical strain has an impact on the energetics of adsorption and transition states of chemical reactions on surfaces. Therefore, it is possible to tune the reactivity by changing the lattice parameter of the catalyst's surface. Since the interaction of hydrogen with iridium surfaces is relevant for a wide range of catalytic reactions, H/Ir(111) was chosen as a model system.

We use density functional theory (DFT) in conjunction with the cluster-expansion method to investigate the energetics of hydrogen adsorption on Ir(111) and its response to strain. DFT data for various configurations with different H coverages and adsorption sites serve as input for a cluster expansion. This approach allows for an exhaustive scan of the configuration space and thus to identify the most favorable structures as a function of coverage. While top-site adsorption is preferred, the system exhibits only a weak tendency for ordering. Moreover, biaxial strain in the surface plane is applied to different configurations to elucidate the correlation between adsorption energies and mechanical strain. In order to gain further insight into the underlying mechanisms, we also analyze the adsorbate induced work function change and its relation to charge transfer.

O 49.12 Tue 18:15 Poster E

High precision structuring of plan and cylindrical metal surfaces of for printing and packaging applications — •Lukas Bayer[1], Mario Gattner[2], Pierre Lorenz[1], Martin Ehrhardt[1], Klaus Zimmer[1], and Michael Mäser[3] — [1]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany — [2]Beuth Hochschule für Technik Berlin University of Applied Science, Luxemburger Straße 10, 13353 Berlin, Germany — [3]SWG, Badstraße 9, 09669 Frankenberg, Germany

Advanced printing and packaging technologies request improvements in resolution and quality as well as in environmental sustainability due to applications for functional surfaces, security printing and advertising. The conventional laser-based production of such tools is subjected to melting effects causing strongly limited results and cost-intensive post processing. Hence, ultra-short laser pulses were used for engraving that can reduce or eliminate those problems. However, high power 1064 nm ps-laser sources must be combined with high speed scanning to avoid heat accumulation and particles shielding. Finally two applications are presented to demonstrate the possibilities of laser engraving. The first shows the production of high quality intaglio printing plates. Here not only the plates but also the printing results are investigated. The second application is the production of laser-induced periodic surface structure (LIPSS). This ripple structures can be produced in short time on large scale cylinders and the distinct optical diffraction effect of the resultant structures can be used for different applications.

O 49.13 Tue 18:15 Poster E

Design and installation of a thermal hydrogen atom source — •Marie Schmitz[1], Dominique Krull[1,2], Christoph Keutner[1,2], Philipp Espeter[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund, Germany

We report on the design and installation of a thermal hydrogen atom source.

The source includes a tungsten capillary, heated radiatively by electron bombardement.

Hydrogen atoms are of substential interest in suface science, especially for thin layer experiments, semiconductor materials science, and technology.

Atomic hydrogen is not only used for surface cleaning, but also to cover surfaces in studies of adsorption, recombination, and desorption. Furthermore, it is crutial for growing layers within thin film deposition.

In this study, the hydrogen source is installed in a UHV-chamber for experimental analysis of adsorption and interaction on Si(100) surfaces, observed by scanning tunneling microscopy (STM). It can also be used for the passivation of Si-substrates. A residual gass analyser is used to assess the performance of the source.

O 50: Overview Talk: Ulrich Höfer

Time: Wednesday 9:30–10:15 Location: S054

Invited Talk O 50.1 Wed 9:30 S054

Shedding light on internal interfaces — •Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg

Electron spectroscopies and scanning probe microscopies have been decisive in bringing surface science to today's high level of understanding. In modern materials science, buried internal interfaces between two solids have become increasingly important. For their investigation, photon-based experimental techniques play a key role.

In this talk, I will discuss perspectives and challenges of the research on internal interfaces and present results obtained for different model systems. For the lattice-matched polar/nonpolar semiconductor interface GaP/Si(001), atomically resolved structural data are available from transmission electron microscopy (TEM). Time-resolved optical second-harmonic generation (SHG) and coherent phonon spectroscopy provide rich information about the dynamics of charge carrier transfer, electric fields and electron-lattice excitations at this interface. Many organic semiconductors can be grown on single crystal metal substrates to form well-defined, atomically abrupt interfaces. Buried only below a few monolayers, these interfaces can be accessed by two-photon photoemission (2PPE). It will be shown that interfaces-specific electronic states are formed for a wide class of such systems. Located between the metallic Fermi level and the molecular LUMO, they efficiently mediate the charge transfer at organic/metal contacts.

Work performed in the framework of the Collaborative Research Centre "Structure and dynamics of internal interfaces" (SFB 1083).

O 51: Organic-Inorganic Systems II: Energy Level Alignment

Time: Wednesday 10:30–13:00 Location: S054

Invited Talk O 51.1 Wed 10:30 S054

Energy level alignment mechanisms at hybrid inorganic/organic semiconductor interfaces — •Norbert Koch — Humboldt-Universität zu Berlin, Berlin, Germany — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Understanding the energy level alignment at hybrid inorganic/organic semiconductor interfaces is indispensable to devise methods that allow for level control. This is needed to achieve a desired functionality of that heterostructure, as for instance, a type-II alignment facilitates charge separation while a type-I alignment is suitable for energy transfer and radiative recombination. For the inorganic semiconductors ZnO and GaN, the use of interlayers, based on strong molecular acceptors and donors, can be employed to tune the energy level alignment with respect to an organic semiconductor deposited on top. Depending on the level alignment achieved in this way, the hybrid heterostructure functionality, e.g., energy or charge transfer, can be selected. Finally, the impact of the doping level of the semiconductors on interface energetics is discussed for a prototypical hybrid p-n-junction.

O 51.2 Wed 11:00 S054

Work Function Increase of GaN and the Influence of Surface Gap States — •Thorsten Schultz[1], Raphael Schlesinger[1], Jens Niederhausen[1,2], and Norbert Koch[1,2] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany

The two molecular organic acceptors HATCN and F6-TCNNQ were vacuum-deposited on non-intentionally doped GaN (0001), which had a residual donor concentration of 1016 cm-3. By means of ultraviolet photoelectron spectroscopy, a huge work function increase (up to 1.5 eV for HATCN and 1.7 eV for F6-TCNNQ) was observed for monolayer coverage, which stems mostly from an interface dipole between substrate and molecules. The contribution of band bending within GaN (ca. 0.35 eV, as determined from X-ray photoelectron spectroscopy) was found to be significantly smaller than expected from theoretical calculations that predict the contribution of band bending to be dominating for low doping concentrations. A qualitative model is introduced, which assigns the low band bending contribution to the presence of substrate surface gap states. These states donate electrons to the acceptor molecules, so less charge is transferred from the GaN donors. This results in less band bending change than expected from calculations, which did not take surface states into account. Our investigations show that the energy level tuning scheme via acceptor interlayers, already successfully employed for ZnO, holds great promise for GaN as well.

O 51.3 Wed 11:15 S054

Structure and stoichiometry prediction of zinc oxide surfaces — •Philipp Herrmann, Navid Abedi Khaledi, and Georg Heimel — Institut für Physik, Humboldt Universität zu Berlin, Germany

Despite their great potential as transparent electrodes in organic electronics and as integral, active components in hybrid (opto-)electronic devices, full control over the surfaces of transition-metal oxides has remained elusive. Atomistic details of their structure and stoichiometry have proven hard to assess, rendering application-relevant surface properties, such as the work function, highly dependent on environment and preparation conditions.

Here, on the example of zinc oxide, I will present a revised approach to the *ab-initio* prediction of atomistic surface structure and stoichiometry as a function of environmental conditions, specifically temperature and atmospheric composition. The predicted structures will be discussed in terms of their experimental signatures in photoelectron spectroscopy, notably surface core-level shifts and work function.

This work thus paves the way for the targeted *in-silico* design of functional inorganic/organic hybrid interfaces.

O 51.4 Wed 11:30 S054

Density-Matrix Derived van der Waals Interactions: Many-Body Dispersion goes Mesoscale — •Martin Stöhr[1,2], Georg Michelitsch[1], John Tully[2], Karsten Reuter[1], and Reinhard Maurer[2] — [1]Technische Universität München — [2]Yale University

The applicability of highly accurate quantum chemical simulation methods is limited to systems of small to moderate size. Density-Functional Theory (DFT), but also more approximate, semi-empirical methods such as Density-Functional based Tight-Binding (DFTB) have shown great success in addressing systems at longer time and length scales. However, a severe drawback of DFTB and many prevalent DFT functionals is the neglect of dispersion interactions, which is particularly consequential for the simulation of e.g. hybrid inorganic-organic systems. Here, we propose a novel approach to obtain effective C6 coefficients in the context of the Tkatchenko-Scheffler dispersion correction scheme [1]. The modified scheme derives atomic dispersion parameters directly from the density-matrix and is thus readily applicable to both full DFT and semi-empirical methods like DFTB, where the electron density is not explicitly constructed. At a fraction of the computational workload of a density-based approach, the scheme yields equally accurate dispersion energies up to the many-body dispersion level for intermolecular interactions in gas-phase and molecular crystals. We exemplify the robustness of the scheme by addressing organic-inorganic interfaces with DFTB using a minimal basis set. [1] A. Tkatchenko and M. Scheffler, *Phys. Rev. Lett.* **102**, 073005 (2009).

O 51.5 Wed 11:45 S054

Single molecules of Sexiphenyl on In2O3(111) — •Margareta Wagner[1], Michael Hollerer[2], Martin Sterrer[2], Michael Ramsey[2], Lynn A. Boatner[3], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institut für Angewandte Physik, TU Wien, Österreich — [2]Institut für Physik, Karl-Franzens-Universität Graz, Österreich — [3]Material Science and Technology Division, ORNL, USA

Indium oxide is one of the most important transparent conductive oxides (TCOs), and commonly used as a contact material. Sexiphenyl (6P) is a rod-like molecule and twice as long as the substrate surface lattice parameter of the (111) surface of In2O3 single crystals.

Here, the adsorption of 6P is investigated with STM. We show that 6P has a specific adsorption site, but no well-ordered monolayer is formed. In empty states STM, the single 6P appears as a zig-zag line at bias voltages below +2V. At +2V the molecule starts to appear straight, which is associated with tunneling into the LUMO state. At +2.7V the apparent shape changes again into two bright features, corresponding to the LUMO+1.

O 51.6 Wed 12:00 S054

Optical transition energies of isolated molecular monomers and weakly interacting 2D aggregates — Roman Forker[1], Thomas Dienel[2], Andreas Krause[3], •Marco Gruenewald[1], Matthias Meissner[1], Tino Kirchhuebel[1], Oliver Gröning[2], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Nanotech@surfaces Laboratory, EMPA - Swiss Federal Laboratories for Materials Science and Technology, Ueberlandstrasse 129, 8600 Duebendorf, Switzerland — [3]NaMLab gGmbH, Noethnitzer Str. 64, 01187 Dresden, Germany

We analyze the $S_0 \rightarrow S_1$ fundamental transition energies observed for 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) as a function of coverage on various surfaces with substantially dissimilar dielectric properties. Surprisingly, only two different spectral positions are found: (i) $\mathrm{PTCDA_{HE}}$ basically mimics the behavior of isolated monomers on the surface, while (ii) $\mathrm{PTCDA_{LE}}$, red-shifted by approx. 70 meV, is attributed to a densely packed monolayer (ML) in a two-dimensional herringbone arrangement. This red-shift is in remarkable accordance with previous investigations for PTCDA on NaCl(100) and thus likely arises from the same physical effects, namely the formation of 2D excitonic bands and the polarizability of neighboring molecules within the ML. Possible contributions from substrate-induced molecular distortions and chemical interactions are discussed. Contrary to earlier studies, we conclude that the polarizability of the substrate is not the dominant factor responsible for the reported spectral positions.

O 51.7 Wed 12:15 S054

Photoemission study of thin films of the singlet fission compound 1,3-Diphenylisobenzofuran — •David Nobis, Janek Rieger, Daniel Niesner, Pedro B. Coto, Michael Thoss, and Thomas Fauster — Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Singlet fission (SF) is the conversion of an optically excited, high-energy singlet exciton, into two optically dark, long-lived electronic excited triplet states via a spin-allowed process. This process might be used in next generation solar cells to harvest high-energy light. 1,3-Diphenylisobenzofuran (DPIBF) is a prototypical SF molecule, as has been shown by calculations and optical spectroscopy [1,2].

We investigated thin films of DPIBF on SiO_2 with UV photoelectron spectroscopy (UPS) and two-photon photoemission (2PPE). The UPS results show the HOMO located 6 eV below the vacuum level, in good agreement with DFT calculations.

The 2PPE spectra show the first singlet state S_1 at 2.8 eV above the HOMO. The triplet state is 1.4 eV lower in energy. Its high, long-lived population is explained by SF in agreement with literature [2].

[1] Schwerin A. F. *et al.*, J. Phys. Chem. A **114** (2010) 1457

[2] Johnson J. C. *et al.*, Phys. Rev. B **132** (2009) 16302

O 51.8 Wed 12:30 S054

Two-photon photoemission from tetraphenylporphyrins on Ag(100) — •Andrej Classen, Rebecca Pöschel, Gianluca Di Filippo, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Ultrathin films of two different tetraphenylporphyrins (2HTPP and MgTPP) were grown in-situ under UHV-conditions on a well-defined Ag(100) single crystal. The molecules were deposited by evaporation from a home-built Knudsen-cell evaporator. The substrate was kept at room temperature and layer thicknesses range from one monolayer of molecules (1 ML) up to multilayer films (19 ML). We present an investigation of the electronic structure using ultraviolet photoelectron spectroscopy and monochromatic two-photon photoemission (2PPE). The occupied molecular orbitals of 2HTPP and MgTPP were measured using a photon energy of 21.22 eV (HeI-radiation). 2PPE probes the unoccupied molecular orbitals. The combination of both yields a HOMO-LUMO gap of 4.2 eV (MgTPP) and 4.3 eV (2HTPP) in accordance with literature [1]. Taking the measured work function into account, the ionization potential is 5.9 eV (MgTPP) and 6.1 eV (2HTPP) [2]. The electron affinity is 1.7 eV (MgTPP) and 1.8 eV (2HTPP). The 2PPE intensity as a function of photon energy in the range from 3.08 eV to 3.38 eV follows the absorption spectrum (Soret band) of tetraphenylporphyrin.

[1] X. Blase et al., Phys. Rev. B **83**, 115103 (2011)

[2] Y. Nakato et al., Chem. Phys. Lett. **39**, 358 (1976)

O 51.9 Wed 12:45 S054

Work function tuning and electrostatic effects: embedded dipoles in aromatic self-assembled monolayers — Swen Schuster[1], Tarek Abu-Husein[2], David A. Egger[3], Iris Hehn[3], Martin Kind[2], Egbert Zojer[3], Andreas Terfort[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, 60438 Frankfurt, Germany — [3]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, 8010 Graz, Austria

Self-assembled monolayers (SAMs) are frequently used as intermediate films to modify charge-carrier injection from metal-electrodes into an organic semiconductor. This is usually achieved by use of the terminal dipolar groups comprising the SAM-ambient interface, affecting, however, the growth chemistry of the semiconductor. Here we suggest an alternative approach, viz. embedding dipolar element into the molecular backbone, decoupling the dipole control and the chemistry at the SAM-ambience interface. In this context, using a representative model system, we studied electronic and structural properties of aromatic SAMs that contain an embedded, dipolar group, viz. pyrimidine. Using a number of complementary characterization techniques combined with quantum-mechanical modeling, we show that such mid-chain substituted monolayers are highly interesting from both fundamental and application viewpoints, as the dipolar groups induce a potential discontinuity inside the monolayer, electrostatically shifting the energy levels in the regions above and below the dipoles relative to one another.

O 52: Photonics and Nanooptics II: Nonlinear Response

Time: Wednesday 10:30–13:15 Location: S051

O 52.1 Wed 10:30 S051

Nonlinear Plasmonic Sensing — •Martin Mesch, Bernd Metzger, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

We introduce the concept of *nonlinear* plasmonic sensing, relying on third harmonic generation from simple plasmonic nanoantennas. Due to the nonlinear conversion process we observe a larger sensitivity upon a local change in the refractive index as compared to the commonly used linear localized surface plasmon resonance sensing. Refractive index changes as small as 10^{-3} can be detected. In order to determine the spectral position of highest sensitivity, we perform linear and third harmonic spectroscopy on plasmonic nanoantenna arrays, which are the fundamental building blocks of our sensor. Furthermore, simultaneous detection of linear and nonlinear signals allows quantitative comparison of both methods, providing further insight into the working principle of our sensor. While the signal-to-noise ratio is comparable, nonlinear sensing gives about seven times higher signal levels. Our scheme can be extended to other nonlinear processes such as second harmonic generation and sum frequency generation. This opens a new avenue in plasmonic sensing.

O 52.2 Wed 10:45 S051

Investigation of Plasmonic Modes of Gold Tapers — •Surong Guo[1], Nahid Talebi[1], Wilfried Sigle[1], Christian Knipl[1], Martin Esmann[2], Simon Becker[2], Ralf Vogelgesang[2], Christoph Lienau[2], and Peter van Aken[1] — [1]Max Planck Institute for Solid State Research , Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]Carl von Ossietzky Universität Oldenburg, Ammerländer Heerstraße 114-118, D-26129 Oldenburg, Germany

Plasmonic tapers have been studied intensively due to the ability of adiabatically coupling the propagating surface plasmon polaritons along their shaft to the nanolocalized plasmons at their apex. Therefore, they can find applications in the fields of sub-diffraction-limit nanofocusing, ultrafast photoemission, and near-field optical microscopy.

We investigate the plasmonic modes of three-dimensional single crystalline gold tapers by means of electron energy loss spectroscopy and numerical calculation. We observe discrete higher-order azimuthal plasmonic modes of the gold taper with an opening angle of ~45° with energy dispersions roughly proportional to the inverse local radius. The importance of phase-matching between electron field and radiative taper modes in mesoscopic structure is demonstrated [1]. We further systematically study the changes in the dispersion of higher-order plasmonic modes of gold tapers versus the opening angle of the taper, both experimentally and theoretically.

[1] N. Talebi et al, ACS Nano, 2015, 9 (7), 7641-7648.

O 52.3 Wed 11:00 S051

Nonlinear Emission of Electrons in a Strong Plasmonic Field — Daniel Podbiel[1], Philip Kahl[1], Bettina Frank[1], Harald Giessen[2], and •Frank Meyer zu Heringdorf[2] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70550 Stuttgart, Germany

Observing surface plasmon polaritons (SPPs) in a photoemission electronmicroscope (PEEM) is possible via nonlinear photoemission if ultra-short laser pulses (<20fs) of a suitable wavelength are directed onto the surface of a plasmonic material. We study the time-resolved propagation and interaction of SPPs by means of a direct conceptual visualization of the SPPs in a "normal incidence geometry". This experimental setup allows us to observe transient phenomena that exist for only a few femtoseconds during the coherent interaction of the ultrashort SPP pulses. In focusing structures for SPPs we find an unexpected time-signature of the nonlinear photoemission signal at the focus point that must be explained by emission of electrons from the SPP alone. The energy distribution of these 'plasmoelectrons' shows that the SPP fields are sufficiently high to make nonlinear photoemission pathways of higher orders the dominant contribution to the PEEM signal.

O 52.4 Wed 11:15 S051

Coherent control of photoemission from a single nanotip in a two-color scheme — •Michael Förster[1,2], Timo Paschen[1], Michael Krüger[1,2], Florian Libisch[3], Christoph Lemell[3], Georg Wachter[3], Thomas Madlener[3], Joachim Burgdörfer[3], and Peter Hommelhoff[1,2,4] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstrasse 1, 91058 Erlangen — [2]Max-Planck Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching — [3]Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstr. 8-10/E136, 1040 Wien — [4]Max-Planck Institut für die Physik des Lichts, Günther-Scharowsky-Str. 1/Geb. 24, 91058 Erlangen

We discuss coherent control of photoemission from a tungsten tip in a Brumer-Shapiro scheme. We observe that photoemission from the nanotip induced by a femtosecond laser displaying many multiphoton orders can be strongly enhanced or reduced by the presence of a weak second harmonic, depending on the phase between the laser pulses. With optimized parameters the phase-dependent contrast in the total emitted current can exceed 90%. Time-resolved data shows that emission takes place on femtosecond time scales. With the help of spectrally-resolved measurements and density functional theory calculations we interpret our observations in terms of interfering emission pathways.

O 52.5 Wed 11:30 S051

Above threshold ionization of Rydberg electrons localized to a gold nanotip — •Jörg Robin[1], Jan Vogelsang[1], Benedek J. Nagy[2], Petra Gross[1], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, 26129 Oldenburg — [2]Wigner Research Centre for Physics, H-1121 Budapest

Metallic nanotips are model systems to study nanometre and femtosecond electron dynamics and provide the possibility for ultrafast electron microscopy. Evidence of strong-field phenomena has been observed by one-colour photoemission of electrons from metallic nanotips [1-3], while two-colour photoemission has established the existence of surface states on metallic films [4]. Here, we report femtosecond two-colour photoemission of electrons from a gold nanotip. We observe long-lived wave packets of Rydberg electrons bound to their own image potential. These intermediate bound states facilitate above-threshold ionization similar to atomic systems and give access to a cold, ultrafast, nanolocalized electron source. [1] Krüger, M. et al. Nature 475, 78 (2011) [2] Herink, G. et al. Nature 483, 190 (2012) [3] Piglosiewicz, B. et al. Nat. Photon. 9, 37 (2014) [4] Höfer, U. et al. Science 277, 1480 (1997)

O 52.6 Wed 11:45 S051

Third harmonic efficiency scaling with plasmonic antenna length — •Maxim Nesterov, Mario Hentschel, Bernd Metzger, Harald Giessen, and Thomas Weiss — 4th Physics Insitute and Research Centre SCoPE, University of Stuttgart, 70550 Stuttgart, Germany

Nonlinear interaction of light with plasmonic structures leads to higher-order harmonic generation, such as second-order harmonics in non-centrosymmetric media, and third-order harmonics in centrosymmetric systems. Metallic antennas are characterized by a high field concentration at resonances, resulting in a relatively strong nonlinear optical response. The enhancement of higher-order harmonic generation depends on the size and shape of antenna, and a strong nonlinear signal can be achieved with a proper design.

We study scaling of the third harmonic generation with rod antenna length numerically for a single antenna, as well as for array configurations. The third-harmonic intensity is found to be increasing as a twelfth power of an antenna length in the model based on Miller's rule. We discuss applicability of the Miller's rule in the context of the origin of the nonlinear susceptibility in the metals. An analytical model has been developed to support the numerical results.

O 52.7 Wed 12:00 S051

Nonlinear chiral plasmonics: Quantitative modeling of the third-harmonic response of 3D chiral plasmonic nanoantennas — •Lili Gui, Xinghui Yin, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

Optical activity exists generally in nature, as many biomolecules such as proteins are chiral. Chiral plasmonic nanostructures are highly interesting since they are potentially ideal and sensitive platforms for biosensing due to the strong superchiral near fields and their own giant chiroptical effects. Exploration of nonlinear chiroptical effects in chiral plasmonic structures is even more desired since the nonlinear chiroptical effects are typically orders of magnitude higher than the linear optical counterparts. Here we study the third-order nonlinear chiroptical effects of 3D chiral structures consisting of corner-stacked gold nanorods. Compared to second-order effects, third-order effects are more immune to fabrication defects and surface roughness. We experimentally investigate the third-harmonic spectroscopy with left- and right-circularly polarized fundamental light, respectively. The third-order chiroptical responses can be well understood when we utilize a coupled anharmonic oscillator model considering the phase retardation of light interaction with the 3D gold nanorods. This model is instructive to guide a practical design of plasmonic chiral structures for a giant third-harmonic-generation circular dichroism (THG-CD) effect.

O 52.8 Wed 12:15 S051

Shaping the Nonlinear Near-Field of Single Gold Nanostructures — •Daniela Wolf[1,2], Julian Obermeier[1], Thorsten Schumacher[1], and Markus Lippitz[1] — [1]Experimental Physics III, University of Bayreuth, Universitaetsstr. 30, 95447 Bayreuth, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Light scattering at plasmonic nanoparticles and their assemblies has led to a wealth of applications in metamaterials and nanooptics. While the shaping of fields around nanostructures is widely studied, the influence of the field inside the nanostructures is often overlooked. The linear field distribution inside the structure taken to the third power causes third-harmonic generation, a nonlinear optical response of matter. Here we demonstrate by a far-field Fourier imaging method how this simple fact can be used to shape fields around already a single particle alone. We employ this scheme to switch the third-harmonic emission from a single point source to two spatially separated but coherent sources, as in Young's double slit assembly. Finally, we present some recent results on more advanced structures combining nonlinear plasmonics and waveguiding.

O 52.9 Wed 12:30 S051

An ultrafast nanotip electron gun triggered by grating-coupled surface plasmons — •Benjamin Schröder, Murat Sivis, Reiner Bormann, Sascha Schäfer, and Claus Ropers — 4th Physical Institute - Solids and Nanostructures, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We present recent results on the photoelectron emission from metal nanotips induced by propagating surface plasmon polaritons (SPPs) excited in a grating-coupler on the tip shaft [1-3]. Nanofocusing of the SPPs induces multiphoton photoemission with high efficiency. The nanostructure is inserted in a modified field-emitter electron gun geometry controlling the electrostatic environment of the tip. In this way, a site-selective control of the electron emission is achieved, and we can disentangle electrons emitted from the apex from those originating at the grating or shaft. Both the control of the transverse beam properties and the local extraction fields enabled by the gun design will be beneficial in future ultrafast transmission electron microscope applications [4].

[1] C. Ropers, C.C. Neacsu, T. Elsaesser, M. Albrecht, M.B. Raschke, and C. Lienau, Nano Lett. 7, 2784 (2007).

[2] S. Berweger, J.M. Atkin, X.G. Xu, R.L. Olmon, and M.B. Raschke, Nano Lett. 11, 4309 (2011).

[3] J. Vogelsang, J. Robin, B.J. Nagy, P. Dombi, D. Rosenkranz, M. Schiek, P. Groß, and C. Lienau, Nano Lett. 15, 4685 (2015).

[4] B. Schröder, M. Sivis, R. Bormann, S. Schäfer, and C. Ropers, accepted for puplication in Appl. Phys. Lett. (2015).

O 52.10 Wed 12:45 S051

Plasmon dynamics on nanoporous gold particles revealed by strong field photoemission — Germann Hergert[1], •Jan Vogelsang[1], Jörg Robin[1], Petra Gross[1], Dong Wang[2], Peter Schaaf[2], Erich Runge[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Technische Universität Ilmenau, Ilmenau, Germany

Nanoporous gold particles or "nanosponges" are particles with a diameter of hundreds of nanometers, perforated with randomly arranged pores with diameters in the 10-nm range. They have recently attracted attention as templates for surface-enhanced Raman sensing as they combine several advantageous properties, such as multiple plasmon resonances in the visible or NIR spectral range, a high surface-to-volume ratio, and a high density of catalytic sites [1].

Here we investigate the plasmon dynamics of such particles using ultrafast photoemission microscopy. When using 14-fs excitation pulses at 1600 nm for excitation of single nanosponges, we observe long-lived plasmon oscillations as a function of the pulse delay. Introducing a new model for the optical properties of these particles, we show that our results reveal the existence of long-lived plasmon hotspots with lifetimes of several tens of fs on the surface of the sponge. This plasmon localization could be of key importance for enhancing the sensing capability of such particles.

[1] C. Vidal et al, ACS Photonics 2, 1436 (2015)

O 52.11 Wed 13:00 S051

Suppression of radiative damping and enhancement of second harmonic generation in bull's eye nanoresonators — •Vladimir Smirnov[1], Jue-min Yi[1], Xianji Piao[2], Jiho Hong[2], Heiko Kollmann[1], Martin Silies[1], Wei Wang[1], Petra Gross[1], Ralf Vogelgesang[1], Namkyoo Park[2], and Christoph Lienau[1] — [1]University of Oldenburg, Germany — [2]Seoul National University, Korea

Bull's eye (BE) nanoresonators, consisting of a central aperture in an Au film surrounded by a series of concentric circular grooves, are highly interesting structures in the context of manipulating light propagation [1] and also optimizing the coupling to quantum emitters [2]. Using broadband linear spectral interferometry and ultrahigh time resolution spectroscopy, we study the temporal response and the local field enhancement of such BE nanoresonators. We find surprisingly long lifetimes of the extended resonator eigenmodes of more than 35 fs [3]. Furthermore, by replacing the central circular hole with an annular ring void, we obtain 50-times higher second harmonic generation efficiency, illustrating the efficient field enhancement and confinement possible in BE nanoresonators. The combination of spatial light concentration with high quality factors has high potential for sensing and coherent control of light-matter interactions on the nanoscale.

[1] H. J. Lezec et al., Science 297, p. 820 (2002); [2] A. G. Curto et al., Science 329, p. 930 (2010); [3] J. Yi et al, submitted to ACS Nano (2015)

O 53: Focus Session: Electrocatalytic Energy Harvesting and Conversion

Time: Wednesday 10:30–13:15 Location: S052

Topical Talk O 53.1 Wed 10:30 S052

Insights into Oxygen Evolution Electrocatalysis on Perovskites — •Thomas J. Schmidt — Electrochemistry Laboratory, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland — Laboratory of Physical Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland

Oxygen electrodes are playing a key role in electrochemical energy conversion devices such as fuel cells and water electrolyzers. In both acidic and alkaline environment, both the oxygen reduction and oxygen evolution reaction (ORR / OER), respectively, are limiting the overall energy/voltage efficiency due to its sluggish kinetics. [1, 2]

Whereas in acidic environment, mainly precious metals are used to catalyze the OER, the variety of possible catalysts in alkaline electrolyte is significantly increased and also many non-noble metal oxide based systems can be employed. Generally, the oxygen evolution mechanisms are only partly understood independent of the electrolyte environment and material used. In order to help to understand the underlying mechanisms for the reactions and to support the experimental results, very often computational methods are used, mainly using density functional theory (DFT) calculations.

In this talk, some of your recent findings on non-noble metal catalysts, mainly from the perovskite family will be presented employing both electrochemical as well as operando spectroscopic techniques.

[1] A. Rabis, P. Rodriguez, T.J. Schmidt, ACS Catal., 2012, 2 (5), 864-890 [2] E. Fabbri, A. Habereder, K. Waltar, R. Kötz, T.J. Schmidt, Cat. Sci. Tech., 2014, 4, 3800-3821

Topical Talk O 53.2 Wed 11:00 S052

Using redox agents to enhance the performance of lithium-air batteries and lithium recycling — •Nuria Garcia-Araez — University of Southampton

Lithium-air batteries can become the next generation of battery technologies, since they can potentially deliver 5 times more energy than current lithium-ion batteries of the same weight, while having a lower cost and being more environmentally friendly. Unfortunately, the performance of the current lithium-air batteries is limited by three fundamental issues: electrode passivation, degradation reactions and poor kinetics of the desired reactions. Luckily, this talk will show that all these issues can be solved by incorporating suitable redox agents, which can act as shuttles and mediators. As the performance of lithium batteries improves, and the global population increases, the demand for lithium can only increase in the future, and therefore lithium recycling and recovery will need to be developed. This talk will also present a new method for lithium recycling that is based on the combination of redox agents and battery materials.

Topical Talk O 53.3 Wed 11:30 S052

Probing the Femtosecond Dynamics of the Hydrogen Evolution Reaction on Gold — •R. Kramer Campen, Francois Lapointe, and Yujin Tong — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

While water electrolysis on gold electrodes was first demonstrated more than 225 years ago, the mechanisms of both the oxygen and hydrogen evolution halves of this process are still controversial. From an experimental point of view part of the challenge has been a lack of methods that allow characterization of transient intermediates. Here we report a novel experimental approach in which we initiate hydrogen evolution at a gold/liquid water interface using an intense, femtosecond, UV pulse to promote an electron from gold's fermi level into water's conduction band and track the fate of this electron with fs time resolution both optically, using interface specific sum frequency generation spectroscopy, and electrochemically via a double-pump, laser induced perturbation of the open circuit potential. The results of this approach suggest that, at circum-neutral pH, (i) at the gold/water interface the delocalized, conduction band, solvated electron has a lifetime of 150-250 fs depending on surface potential (ii) conduction band electrons relax to form localized solvated electrons the great majority of which have a potential dependent lifetime of 1-18 ps while a small fraction live for much longer, > 40 ps, and drive chemistry. These results furnish a potential-dependent, mechanistic picture of the transfer of electrons from gold into liquid water, the first step in hydrogen evolution.

15 min. break

Topical Talk O 53.4 Wed 12:15 S052

The Electrochemical interface - at the atomic scale — •Jan Rossmeisl — Department of Chemistry, Nano-science center, University of Copenhagen Universitetsparken 5, 2100, København Ø, Denmark

There are presently no atomic scale simulations or analysis that capture all the essential parts of the nature electrochemical interface. Thus the electrochemical solid/liquid interface represents one of the frontiers of atomic scale simulations. The electrolyte is as important for the fundamental properties of the interface as the surface. The challenge is to model the effect of and interplay between potential, pH and ion strength. Thus far these effects have not correctly been accounted for. However, based on a thermochemical analysis it is now possible to account for the effect of pH and ions in the electrolyte on the atomic structure of the interface.

Topical Talk O 53.5 Wed 12:45 S052

CO2 Electroreduction over Cu and Au Nanostructured Catalysts: Size, Oxidation State and Interparticle Distance Effects — Hemma Mistry[1,2], Rulle Reske[3], Farzad Behafarid[2], Ana Sofia Varela[3], Peter Strasser[3], and •Beatriz Roldan Cuenya[1] — [1]Department of Physics, Ruhr-University Bochum, 44708 Bochum, Germany — [2]Department of Physics, University of Central Florida, Orlando FL 32816, USA — [3]Department of Chemistry, Chemical Engineering Division, Technical University Berlin, 10623 Berlin, Germany

The electrocatalytic reduction of CO2 to industrial chemicals and fuels is a promising pathway to sustainable electrical energy storage and to an artificial carbon cycle, but is currently hindered by the low energy efficiency and activity displayed by traditional electrode materials. The structure-dependent catalytic activity of Cu and Au nanoparticle (NP) catalysts for the electroreduction of CO2 is reported here. NPs with well-defined size and interparticle distance were synthesized, and their activity and selectivity measured. A drastic increase in current density was observed with decreasing Au NP size, along with a decrease in selectivity towards CO. Cu NP catalysts also displayed a significant increase in the catalytic activity and selectivity for H2 and CO with decreasing NP size, while methane and ethylene selectivity was increasingly suppressed. The size dependent trends observed can be rationalized by the increased population of low-coordinated surface sites on smaller NPs. The selectivity of Cu NP catalysts could be tuned by varying the interparticle distance due to mass transport phenomena such as reactant diffusion and readsorption of intermediates.

O 54: 2D Materials II: Growth

Time: Wednesday 10:30–13:00 Location: S053

O 54.1 Wed 10:30 S053

Growth and electronic structure of epitaxial single-layer WS_2 on Au(111) — •Maciej Dendzik, Matteo Michiardi, Charlotte Sanders, Marco Bianchi, Jill A. Miwa, Signe S. Grønborg, Jeppe V. Lauritsen, Albert Bruix, Bjørk Hammer, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

Single-layer WS_2 is a promising alternative to the widely studied MoS_2, because of the larger size of the spin-splitting and the lower effective mass of the valence band maximum. Here we present a detailed study of the electronic structure of the large-area single-layer WS_2 grown epitaxially on Au(111) using evaporation of W atoms in a low pressure H_2S atmosphere. The growth process is characterized by means of scanning tunneling microscopy, low-energy electron diffraction and core-level spectroscopy. The electronic band structure of the single-layer WS_2 is determined by angle-resolved photoemission spectroscopy. The valence band maximum at $\bar{K}$ is found to be significantly higher than at $\bar{\Gamma}$. The observed dispersion around $\bar{K}$ is in good agreement with density functional theory calculations for a free-standing monolayer, whereas the bands at $\bar{\Gamma}$ are found to be hybridized with states originating from the Au substrate. Strong spin-orbit coupling leads to a large spin-splitting of the bands in the neighborhood of the $\bar{K}$ points, with a maximum splitting of 419(11) meV. The valence band dispersion around $\bar{K}$ is found to be highly anisotropic with spin-branch dependent effective hole masses of $0.40(02)m_e$ and $0.57(09)m_e$ for the upper and lower split valence band, respectively.

O 54.2 Wed 10:45 S053

Synthesis of high quality TaS_2 monolayer using molecular beam epitaxy — •Arlette S. Ngankeu, Charlotte E. Sanders, Marco Bianchi, Maciej Dendzik, and Philip Hofmann — Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

The transition metal dichalcogenide TaS_2 has been intensively studied in its bulk form due to the rich properties arising from the interplay of electronic instabilities. As in many other materials, the electronic properties of TaS_2 might change in interesting ways in the thickness limit of a single layer. However, finding a good method for the production of high quality single layer TaS_2 is still a big challenge, and the thinnest crystals of TaS_2 obtained so far (by exfoliation of the TaS_2 bulk) actually have thicknesses of a few monolayers. In this talk, we report the first successful preparation of single- and few-layered TaS_2 on the Au(111) substrate by molecular beam epitaxy. Scanning tunneling microscopy, low energy electron diffraction and angle resolved photoemission spectroscopy have been used to probe the surface topography and electronic properties of TaS_2/Au.

O 54.3 Wed 11:00 S053

2D Heterojunctions from Non-local Manipulations of the Interactions — Malte Rösner[1,2], •Christina Steinke[1,2], Michael Lorke[1], Christopher Gies[1], Frank Jahnke[1], and Tim O. Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany

We propose to create lateral heterojunctions in homogeneous two-dimensional materials based on non-local manipulations of the Coulomb interaction using structured dielectric substrates. By means of ab-initio calculations for MoS_2 as well as generic semiconductor models, we show, that changes in the dielectric environment can induce sizeable band-gap modulations. The Coulomb interaction induced self energy corrections in real space are sufficiently non-local, to be manipulated externally, and are clearly localized within a radius of a few unit cell at the same time. This allows to induce spatially sharp interfaces within a single homogeneous monolayer and thus to form a heterojunction by the external manipulation of the Coulomb interaction via structured dielectric substrates. Hence, new kinds of heterojunctions can be constructed by placing semiconducting 2d materials on appropriately structured substrates: For a laterally structured dielectric environment, we find a type-II heterojunction with a sharp band-gap crossover within less than 5 unit cells. By establishing four perpendicular interfaces a band gap modulation reminiscent of a quantum dot can be realised.

O 54.4 Wed 11:15 S053

TFT Fabrication Based on Liquid Exfoliated MoS_2 Flakes — •Xiaoling Zeng[1], Sonia Metel[2,3], Valeria Nicolosi[2,3,4], and Veit Wagner[1] — [1]Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany — [2]School of Chemistry, Trinity College Dublin, Ireland — [3]CRANN, Trinity College Dublin, Ireland — [4]School of Physics, Trinity College Dublin, Ireland

There is a large interest in establishing cheap, scalable processes for producing low dimensional semiconducting dichalcogenide films for electronic application. In this work, well exfoliated MoS_2 dispersions were prepared through two step liquid phase exfoliation process with N-methyl-pyrrolidone (NMP) and Isopropanol (IPA). The obtained exfoliated MoS_2 flakes were characterized by microscopy (TEM and SEM), Uv - Vis and Raman spectroscopy.

Bottom gate thin film transistors (TFTs) based on exfoliated MoS_2 film were fabricated by using spray coating techniques. The deposition process was optimized to get uniform and percolated MoS_2 film with different thicknesses. Transistors show only minor conductivity directly after layer deposition. However, depositing additional PMMA layer on top shows large improvement in electrical characteristics, i.e. switching behavior with changing gate voltage. Interpretation is that the PMMA layer brings the initially separated flakes into contact and enables proper percolation. Further investigation found that the thickness of PMMA influences the electrical properties. This low-cost and scalable solution-based fabrication process will promote the application of dichalcogenides in future nanoelectronic devices.

O 54.5 Wed 11:30 S053

Novel Deposition Approach of Semiconducting MoS2 Thin Films and Their Application for Electronic Devices — •Francis Oliver Vinay Gomes[1,2], Marko Marinkovic[1], Jochen Brendt[1], Torsten Balster[2], and Veit Wagner[2] — [1]Evonik Resource Efficiency GmbH, Paul-Baumann-Strasse 1, 45764 Marl, Germany — [2]Jacobs University Bremen, Department of Physics & Earth Science, Campus Ring 1, 28759 Bremen, Germany

In this work, MoS2 films obtained from precursor solution via spin-coating on various substrates were investigated. Molybdenum(V) chloride dissolved in 1-methoxy-2-propanol was used as precursor solution. The MoS2 films obtained from the Mo-precursor upon sulfurization during annealing were analyzed for surface morphology and roughness, chemical composition and crystallinity. In addition, comparison of silicon and sapphire substrates were studied. Our approach focuses on novel deposition technique compared to the current state-of-the-art chemical vapour deposition.

The thickness of the MoS2 films was controlled in the process, and film thicknesses between 2 and 27 nm were obtained. The thickness of the films linearly scaled with precursor concentration. SEM/EDX measurements indicate that the surface morphology and film composition is strongly dependent on the annealing temperature and processing environment. Electrical measurements demonstrate a film conductivity of 0.27 S/cm while XRD confirms the formation of semiconducting 2H-MoS2 films. The future steps will lead towards applying fabricated films in electronic devices such as thin film transistors.

O 54.6 Wed 11:45 S053

Growing graphene underneath hBN on Rh(111) — •Uta Schlickum[1], Daniel Rosenblatt[1], Sebastian Koslowski[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The stable hexagonal monolayer of hBN is an insulator with excellent dielectric properties. It can be grown on a large variety of transition metal surfaces like Rh(111) on which it shows a hexagonal Moire super-lattice. We grow a single layer of hBN on Rh(111) by chemical vapor deposition and found beside the well known hexagonal structure a new periodic pattern resembling a lattice of a "spoked wheel" (SW). For small coverages this new phase appears at the intersection of the rims connecting three valleys of the Moire lattice, and forms large islands for higher coverage. Atomic resolution topographic images reveal that the phase boundaries do not disturb the atomic lattice periodicity of the hBN. Depending on the preparation parameters, the relative coverage of the two phases can be tuned at will. The crucial parameter determining the relative coverage is the time, the sample stays at about $600°C$ after the exposure to borazine at $800°C$. It is well known that at $600°C$, C impurities segregate and accumulate at the surface. This together with the fact that the hBN lattice itself remains intact crossing a phase boundary, leads us to conclude that the SW phase consists of an additional graphene layer below the hBN layer. Various experimental details, like high resolution spectroscopy, support this interpretation.

O 54.7 Wed 12:00 S053

Prediction of metastable two-dimensional compounds in the C/Si system using global optimization techniques, and investigation of their electronic properties — •Johann Christian Schön and Rico Gutzler — MPI for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart

We employ the global energy landscape exploration package G42+[1,2] to predict (meta)stable two-dimensional crystalline polymorphs in the carbon/silicon system for a range of compositions: C:Si = 1:0, 3:1, 2:1, 1:1, 1:2, 1:3, and 0:1.[1] During the global search (energy function: DFT), both atom positions and cell parameters in the xy-plane were allowed to vary freely. The global optimization method used was basin-hopping-simulated annealing, with two consecutive local optimizations - the first keeping the atoms restricted to the z = 0 plane, while the second one also permitted relaxation in the z-direction. For all compositions, the lowest energy 2D-structures exhibited a graphene-like super-structure with 6-membered rings, but many quite stable competing minimum structures containing a variety of rings of size 4 - 12 were also observed. Deviations from planarity occurred most frequently for structures where a high local concentration of the Si-atoms was present. Complementing geometric structure prediction, we performed band-structure calculations to investigate the effect of geometry and C:Si ratio on the electronic properties of these 2D-materials.

[1] J. C. Schön, Proc. Appl. Ceram. 9:157-168 (2015); [2] J. C. Schön, G42+ Manual, www.chemie.uni-bonn.de/ac/schoen/forschung/g42-manual, (2015)

O 54.8 Wed 12:15 S053

Tuning the physical properties of MoS_2 membranes by organophosphonate interfacial chemistry — •Susanne Schwarzwälder[1], Réka Csiki[1], Eric Parzinger[1], Jeffrey Schwartz[2], Alexander Holleitner[1], Martin Stutzmann[1], Ursula Wurstbauer[1], and Anna Cattani-Scholz[1] — [1]Walter Schottky Institut and Physik Department, Technische Universität München, Germany — [2]Princeton University, New Jersey, USA

One of the most prominent members of the 2D material family is the transition metal dichalcogenide MoS_2, due to its natural occurrence and its promising potential applications in nanoelectronic and optoelectronic devices [1]. Interfacial chemistry strongly influences the interaction of molecularly thin semiconducting membranes with the underlying substrate, hence a suitable silicon surface functionalization can be employed for improving the performance of MoS_2-based devices [2]. Our work focuses on the investigation of surface functionalization using homogeneous organophosphonate self-assembled monolayers (SAMs) covalently bonded to SiO_2. In particular, the interaction of single layer (SL) MoS_2 with SAMs based on four different aromatic phosphonic acids are investigated. Modulation of the intrinsic n-type doping of SL-MoS_2 via charge transfer with aromatic SAMs is suggested by a shift in the Raman-active out-of plane vibrational mode A_{1g}, emphasizing the importance of interfacial interactions in MoS_2-based nanodevices.

[1] R. Ganatra, Q. Zhang, ACS Nano 8, 4074 (2014).

[2] S. Najmaei et al., Nano Lett. 14, 1354 (2014).

O 54.9 Wed 12:30 S053

Structural analysis of one monolayer of hBN on Cu(111) via NIXSW and SPA-LEED — •Timo Heepenstrick[1], Christine Brülke[1], Ina Krieger[1], Sergey Subach[2], Simon Weiss[2], Niklas Humberg[1], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52452 Jülich, Germany

We present a detailed structural analysis of hBN on Cu(111) with normal incidence x-ray standing waves (NIXSW) supported by spot profile analysis low energy electron diffraction (SPA-LEED). hBN forms an incommensurate structure on Cu(111) with a lattice mismatch of 2.3% corresponding to the unstrained hBN layer. The NIXSW experiments show that the hBN layer is weakly bonded with a distance of 3.23 Å (for the nitrogen) and 3.26 Å (for the boron) and shows little buckling. We also present an analysis for the topmost Cu(111) layer with and without a monolayer of hBN.

O 54.10 Wed 12:45 S053

Nanotents - 2 nm void-formation and self-healing in 2D monolayers on metals — •Huanyao Cun[1], Marcella Iannuzzi[2], Adrian Hemmi[1], Silvan Roth[1], Jürg Osterwalder[1], and Thomas Greber[1] — [1]Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [2]Chemistry-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

At room temperature, it is quite challenging to immobilize single atoms. However, with the single layers of hexagonal boron nitride (h-BN) or graphene, site-selective immobilization of atoms at surfaces becomes feasible. The h-BN nanomesh is a corrugated structure that consists of two regions, the 'pores' with 2 nm diameter and the surrounding 'wire' regions.

In the present study, we demonstrate that the h-BN nanomesh, which acts as thin "rainfly", can trap atoms at distinct subsurface sites and form so-called "nanotents" structure. Remarkably, annealing to 900 K induces the "can-opener" effect: h-BN flakes at pore sites are cut out from the h-BN monolayer and 2 nm voids form on the h-BN surface. We assign the "can-opener" effect to the vacancy defects generated during the Ar+ penetration. Higher temperature annealing leads to the "self-healing" of the h-BN monolayer. Systematic measurements reveal that the entire process, including nanotent formation, "can-opener" effect and nanomesh "self-healing", is well controlled and repeatable. The reported effects are robust and quite general: they are also observed in graphene on ruthenium, for neon and rubidium atoms.

O 55: Frontiers of Electronic Structure Theory: Focus on Topology and Transport II

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

O 55.1 Wed 10:30 H24

Coupled-Cluster approach for both molecules and solids in the numeric atom-center orbital framework — •Tonghao Shen, Arvid Conrad Ihrig, Igor Ying Zhang, and Matthias Scheffler — *Fritz-Haber-Institut der MPG, Berlin.*

For a quantitative prediction of material properties, an advanced description of electronic correlation is crucial. As the "gold standard" correlation method in quantum chemistry, the coupled-cluster (CC) ansatz with singles, doubles and perturbative triples (CCSD(T)) is starting to gain attention in materials science[1]. At present, the CCSD(T)-quality description of the correlation effects in solids can be achieved by either studying the cluster-size convergence toward the bulk in real space[1] or implementing CCSD(T) for extended systems in reciprocal space[2]. In order to investigate and compare these approaches on an equal footing, it is essential to have a computational platform that enables CCSD(T) simulations to be carried out using both cluster and periodic models in a single computational environment. In this report, we present a CCSD(T) implementation for both molecules and solids in the all-electron full-potential code FHI-aims[3] with numeric atom-center orbital(NAO) basis sets. A special memory-distribution strategy is designed to significantly reduce the inter-CPU communication, which is the main challenge for the parallelization of wave-function methods. The accuracy and efficiency are demonstrated for a group of molecules, 1D-, 2D- and 3D-periodic materials. [1] C. Müller, *et al.*, PCCP. **14**, 7605 (2012); [2] A. Grüneis, *et al.*, JCTC **7**, 2780 (2011); [3] V. Blum, *et al.*, CPC **180**, 2175-2196 (2009).

O 55.2 Wed 10:45 H24

Surface adsorption energetics at the "gold standard": Small molecule binding to $\mathbf{TiO_2(110)}$ — •Daniel Berger[1,2], A. Kubas[3], D. Manganas[3], H. Oberhofer[1], F. Neese[3], and K. Reuter[1] — [1]TU München — [2]University of California, Los Angeles — [3]MPI für chemische Energiekonversion, Mülheim an der Ruhr

Adsorption energies at oxide surfaces are central quantities required for catalysis, energy and a multitude of other application areas. At present, the by far dominant computational method to obtain such energetics is density-functional theory (DFT). Unfortunately, systematic benchmarking of such energetics against accurate reference numbers from correlated wave-function theory as known from molecular systems is scarce, largely owing to the fact that the latter techniques are often not available for standard periodic boundary condition supercell calculations.

We address this situation with a solid-state QM/MM embedded cluster approach, in which the adsorbate and immediate surrounding surface atoms are described quantum mechanically, while the long-range electrostatic interactions are accounted for through a polarizable force field. This yields a numerically highly efficient approach that enables use of the recently developed domain-based local pair natural orbital coupled cluster method with single-, double- and perturbative triple-excitations (DLPNO-CCSD(T)) in the quantum region. We exploit corresponding "gold standard" adsorption energies for a set of prototypical small molecules interacting with the rutile $TiO_2(110)$ surface for a systematic benchmark of DFT numbers.

O 55.3 Wed 11:00 H24

Water adsortpion on surfaces form many-body perturbation theory — •Theodoros Tsatsoulis and Andreas Grüneis — Max-Planck-Institute for Solid State Research, Stuttgart

The accurate description of the interaction of molecules with surfaces is of crucial importance for a wide range of phenomena. While Kohn-Sham density functional theory is one of the most widely-used methods for describing the electronic structure of surfaces, many local and semi-local functionals are often not able to produce accurate molecular adsorption energies. Quantum chemical wave-function based methods such as Møller-Plesset perturbation theory (MP2) and coupled-cluster methods promise controllable accuracy, however, at much higher computational costs. Large part of the latter is due to the number of virtual states. We consider an approach whereby the occupied orbitals are converged in a plane wave basis, whereas the virtual space is then constructed using pseudized Gaussian orbitals expanded in plane waves, leading to reduced computational cost. In particular we study water adsorption on bulk LiH and h-BN sheets at the level of MP2 theory within the projector-augmented-wave method as implemented in VASP [1]. The results are compared to state-of-the-art methods such as hybrid functionals and diffusion Monte Carlo [2].

[1] Marsman et al., The Journal of Chemical Physics, 130, 184103 (2009)

[2] Al-Hamdani et al., The Journal of Chemical Physics, 142, 181101 (2015)

O 55.4 Wed 11:15 H24

Photo-isomerization in azobenzene-functionalized self-assembled monolayers: The impact of many-body effects — •Caterina Cocchi and Claudia Draxl — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Self-assembled monolayers (SAMs) of azobenzene-functionalized alkanethiols on gold suffer from hindered photo-isomerization, as observed experimentally [1]. While this behavior is generally ascribed to strong intermolecular coupling, a clear microscopic understanding of this phenomenon is still missing. In order to address this question, we perform a first-principles study of the excited-state properties of azobenzene-functionalized SAMs. In the framework of many-body perturbation theory (GW approximation and Bethe-Salpeter equation), as implemented in the all-electron full-potential code exciting [2], we investigate the optical absorption spectra of these materials, inspecting the influence of packing density and functionalization of the azobenzene molecules with different end groups. Through a systematic analysis of the character of the excitations, we clarify the role and interplay of screening and local-field effects, which strongly impact light absorption and hence photo-isomerization in these systems.

[1] C. Gahl et al. J. Am. Chem. Soc. 132, 1838 (2010). [2] A. Gulans et al. J. Phys.: Condens. Matter 26, 363202 (2014).

O 55.5 Wed 11:30 H24

Laplace-transformed MP2 with localized Resolution of Identity -efficient in-memory MP2 for large systems — •Arvid Conrad Ihrig[1], Patrick Rinke[2], Igor Ying Zhang[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Aalto University, Helsinki, Finland

A well-known problem in local and semi-local density functional approximations and to a lesser extend also in hybrid functionals is the one-electron self-interaction error, which can lead to a qualitatively wrong description for applications like charge-transfer systems. One possible remedy is the 2nd order Møller-Plesset perturbation theory (MP2), which does not suffer from this error. However, the time and memory requirements for MP2 prevent it routine-use for large molecular and periodic systems. The Laplace-transformed MP2 (LT-MP2) [1] can significantly reduce the computational time, but requires the usage of intermediate variables stored on disk, resulting in an inefficient usage of computational resources. In this work we combine the LT-MP2 with our localized Resolution of Identity (RI-LVL) [2] approach to eliminate the disk-storage bottleneck and fully exploit massive parallelization strategies. RI-LVL expands the basis function pairs in the electron repulsion integrals in local auxiliary basis sets. For the example of water clusters, we demonstrate the favourable memory scaling

(at worst N^2) of our new MP2 implementation, which facilitates the in-memory calculation of large systems at high accuracies.
[1] P. Ayala et al., J. Chem. Phys. 110, 3660 (1999)
[2] Ihrig et al., New J. Phys. 17, 093020 (2015)

O 55.6 Wed 11:45 H24

GW singles contributions for the random phase approximation correlation energies

— •Jiri Klimes[1], Merzuk Kaltak[2], Emanuele Maggio[3], and Georg Kresse[3] — [1]J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic — [2]Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY — [3]University of Vienna, Faculty of Physics, Vienna, Austria

The random phase approximation (RPA) to the correlation energy yields often very accurate results for condensed matter systems. However, a general tendency to underbind has been observed for systems such as molecular solids or for adsorption. One of the ways that have been proposed to improve the accuracy of RPA are the so-called singles corrections of Ren and coworkers [1]. We present our derivation of the singles corrections using the assumption that the electron density changes when going from the reference to the interacting system [2]. This leads to a very compact expression for the corrections. Moreover, the singles formula can be easily modified to account for screening effects, giving the *GW* singles. We assess the effect of both the original and modified singles on covalently and metallically bonded systems as well as on simple weakly bonded systems. Finally, we show that adding the singles corrections leads to considerably improved adsorption energies and lattice energies of molecular solids.

[1] Ren, Tkatchenko, Rinke, Scheffler, Phys. Rev. Lett **106**, 153003 (2010).

[2] Klimeš, Kaltak, Maggio, Kresse, J. Chem. Phys. **143**, 102816 (2015).

O 55.7 Wed 12:00 H24

Long-range corrected DFT meets *GW*: Vibrationally resolved photoelectron spectra from first principles

— •Thomas Körzdörfer — Institut für Chemie, Universität Potsdam, D-14476 Potsdam

We introduce an entirely non-empirical and computationally efficient scheme to calculate highly reliable vibrationally resolved photoelectron spectra for molecules from first principles.[1] To this end, we combine non-empirically tuned long-range corrected hybrid functionals with non-self-consistent many-body perturbation theory in the G_0W_0 approximation and a Franck-Condon multi-mode analysis based on DFT-calculated frequencies. The vibrational analysis allows for a direct comparison of the GW-calculated spectra to gas-phase ultraviolet photoelectron measurements of neutral and anionic molecules, respectively. In addition, vertical IPs and EAs were benchmarked against other *GW* methods and basis-set extrapolated CCSD(T) results for a recently introduced test set of 24 molecules frequently used in organic electronics.[2] G_0W_0@LRC-DFT yields mean absolute errors on the order of 0.1 eV for IPs, EAs, and fundamental gaps, clearly outperforming commonly used G_0W_0 approaches as well as partially and fully self-consistent *GW* methods.
[1] L. Gallandi and T. Körzdörfer, JCTC **11**, 5391 (2015).
[2] L. Gallandi, N. Marom, P. Rinke, and T. Körzdörfer, JCTC *accepted for publication* (2015).

O 55.8 Wed 12:15 H24

LDA-1/2 as a starting point for G_0W_0 calculations

— •Ronaldo Rodrigues Pela[1,2], Ute Werner[1], Dmitrii Nabok[1], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany — [2]Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil

For many semiconductors and insulators, LDA represents a bad starting point for G_0W_0 calculations. Hybrid functionals improve upon LDA, but at the price of increasing computational cost of about 2 orders of magnitude. An alternative starting-point for the single-shot G_0W_0 can be the LDA-1/2 method [1], because it approximately includes the self-energy of quasi-particles within a generalized Kohn-Sham scheme, leading to improved band-gaps over the LDA ones, but without being computationally more involved. In this work, we systematically compare 3 starting-points for G_0W_0 calculations: LDA, PBE0, and the LDA-1/2 method. A selection of semiconductors (C, Si, SiC, AlP, LiF, MgO, Ne, Ar, GaN, GaAs, CdS, ZnS, and ZnO) is chosen for this benchmark. We demonstrate that LDA-1/2 is a good choice in most cases, reducing the root mean square error in band-gap predictions by 50% when compared to G_0W_0 on top of LDA or PBE0. With the exception of large band gap materials, LDA-1/2 predictions are already close to the experimental band gaps, and thus G_0W_0 has minor effects.

Reference [1]: Phys. Rev. B 78, 125116 (2008).

Acknowledgements: “Coordenação de Aperfeiçoamento de Pessoal de Nível Superior” (CAPES) and “Alexander von Humboldt Stiftung”.

O 55.9 Wed 12:30 H24

DFT+U within a numeric atom-centered orbital basis

— •Matthias Kick, Harald Oberhofer, and Karsten Reuter — Technische Universität München

Materials like transition metal oxides (TMOs) still challenge a description through first-principles density-functional theory (DFT). Appropriately capturing the electron localization in TMOs generally requires at least hybrid exchange-correlation functionals. Such higher-rung functionals come with appreciable computational cost, which limits their use in large supercell calculations. For such applications effective and numerically less intense approaches are therefore still a much sought alternative.

One such method is the DFT+U approach, where the on-site Coulomb correlation effects are treated using a model Hamiltonian, while remaining interactions are treated on the level of semi-local DFT. Full DFT+U functionality including nuclear gradients (forces) has been implemented in the electronic structure code *FHI-aims*. We account for three common occupation matrix representations, differing in the way how the occupations of the correlated subspaces are determined. We critically discuss their performance and differences in the context of the numeric atomic orbital basis sets employed in *FHI-aims*. The established numerically efficient framework is finally used to address neutral and charged oxygen vacancies at the TiO_2(110) surface within a solid-state embedding approach.

O 55.10 Wed 12:45 H24

High-throughput Screening and Statistical Learning for Design of Transparent Conducting Oxides

— •Christopher Sutton, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Transparent conducting oxides (TCOs) represent a class of well-developed and commercialized wide-bandgap semiconductors that are crucial for many electronic devices. Ternary Al, Ga, and In-based sesquioxides are investigated as alternative wide-bandgap semiconductors motivated by very intriguing recent experimental work that has demonstrated bandgap engineering in (GayIn1-y)2O3 from 3.8 eV to ca. 5 eV[1] and ca. 5 eV to 7.5 eV for (Al1-xGax)2O3.[2]

New ternary oxides with the chemical structure of (AlxGayIn1-x-y)2O3 have been identified using cluster expansion (CE) models combined with fast stochastic optimization techniques (e.g., Wang-Landau and diffusive nested sampling) in order to efficiently search potential (ordered and disordered) configurations within a given lattice and for different temperatures. Wang-Landau and diffusive nested sampling has also allowed for a consideration of the effect of entropy on the relative stability of ternary oxides. Statistical learning has also been used to identify a structure-property relationship to efficiently identify new wide-band gap TCOs to improve the fundamental chemical and physical properties (e.g., conductivities, mobilities, and optical transparency) by investigating the parameters that control these properties.

[1] F Zhang, et al., Solid State Communications 2014, 186, 28. [2] H Ito, et al., Japanese Journal of Applied Physics 2012, 51, 100207.

O 56: Nanostructures: Dots, Particles and Clusters

Time: Wednesday 10:30–12:30 Location: H4

O 56.1 Wed 10:30 H4

Coherent X-ray Diffraction of Single Epitaxial Nano-Objects — •Thomas F. Keller[1,2], Roman Shayduk[1], Vedran Vonk[1], Arti Dangwal Pandey[1], Claudia Neisser[3], Irene Fernandez-Cuesta[2], Alexey Zozulya[1], Michael Sprung[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany — [2]Institute for Nanostructure and Solid State Physics, University of Hamburg, Germany — [3]Institute for Ion Beam Physics, Helmholtz Center Dresden-Rossendorf, Germany

Controlled nanocatalysis requires novel approaches to understand the size-dependence of catalytic processes. We report on a one-to-one structure analysis of a single platinum (Pt) nanodot-array supported by a strontium titanate STO(100) single crystal by real-space imaging in a scanning electron microscope and in reciprocal space using coherent Bragg diffraction from a focused X-ray beam at PETRA III at DESY.

The Pt nanodot-array was created using a combined lift-off and etching process based on e-beam lithography. Utilizing a transfer and repositioning protocol using the Pt X-ray fluorescence we localized the 2x2 mu^2 array with a center-center distance of 150 nm between single Pt nanodots. The Pt(111) Bragg peak position indicates a preferential Pt(111)/STO(100) orientation. The interference fringes of this peak are typical for coherent diffraction and allow extracting particle shape, size and interparticle distance to compare with the real space imaging.

We propose the use of such nanodot-arrays for future experiments on in-situ oxidation or catalysis as well as for coherent X-ray diffraction of single nano-assemblies under reaction conditions.

O 56.2 Wed 10:45 H4

Cluster mobility of supported size-selected clusters — •Amelie Porzelt, Fabian Knoller, Michael König, Yves Fukamori, Friedrich Esch, and Ueli Heiz — Technische Universität München, Chair of Physical Chemistry, Lichtenbergstr. 4, 85748 Garching, Germany

We present our studies on the ripening dynamics of individual size-selected clusters on a periodically wettable Moiré-graphene film on Rh(111). By imaging the cluster dispersion and by tracking the cluster diffusion, insight into the fundamental processes that govern the cluster diffusion can be gained - how do clusters start their diffusive motion, which path do they follow, how do they stop, and how does this behavior depend on their specific size? We present data on the diffusion of bare clusters and investigate changes induced by adsorbates such as CO, hydrogen or oxygen.

O 56.3 Wed 11:00 H4

Mass selected copper clusters on thin oxide films investigated with STM — •Dominik Wolter[1], Raphael Floegel[1], Matthias Bohlen[1,2], Christoph Schröder[1], Conrad Becker[3], and Heinz Hövel[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Now at: Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany — [3]Aix-Marseille Université, CNRS, CINaM UMR 7325, 13288 Marseille, France

Oxide layers are commonly used for industrial purposes (e.g. microelectronics) but also a topic of current research. It was shown previously, that an Al_2O_3 film on a clean $Ni_3Al(111)$ surface can provide a template for palladium cluster array growth [1]. The quality of the oxidized surface was investigated with **L**ow-**E**nergy **E**lectron **D**iffraction and **S**canning **T**unneling **M**icroscopy. These oxide films are suitable for the deposition and investigation of mass selected clusters, because the layers are thick enough to minimize cluster-surface interaction but simultaneously thin enough to keep characterization with STM feasible. We evaluate the apparent height of deposited copper clusters as well as the next-neighbor distances in order to investigate their arrangement on the oxidized surface. Furthermore the mobility of the clusters is analyzed by incremental heating procedures. The next-neighbor distances can then be compared to Monte Carlo simulation data for various lattices to check whether the clusters attach to the template structure given by the oxide film or not. [1] S. Degen, C. Becker and K. Wandelt, Faraday Discuss., **125**, 343-356 (2004).

O 56.4 Wed 11:15 H4

Towards the geometrical structure of small, deposited Au nanoclusters using grazing incidence X-ray scattering — •Deniza Chekrygina[1], Matthias Schwartzkopf[2], Bjoern Beyersdorff[2], André Rothkirch[2], Ivan Baev[1], Torben Beeck[1], Fridtjof Kielgast[1], Stephan Klumpp[1], Jan-Hendrik Ruescher[1], Stephan Roth[2], Wilfried Wurth[1,2], and Michael Martins[1] — [1]Physik Department, Universität Hamburg — [2]DESY Photon Science, Hamburg

Mass-selected gold clusters deposited on a surface consisting of only a few atoms are of great interest due to their quantum size effects [J.Phys.Chem A, 103,9573 (1999)]. The geometrical structure of these objects is still not determined for most cases and the existing theoretical models are contradictory [Phys.Rev.B 67,085404(2003);Str.Chem., V16,N4(2005)]. In our work we investigate the geometrical structure of size-selected Au9 clusters deposited on a silicon substrate prepared under different soft-landing conditions. The clusters were capped with a thin Al film to suppress oxidation. Due to the very small size of our clusters we follow a new path for structural analysis. We compare differently prepared samples and present first results obtained using a combination of several complimentary methods performed in parallel: Grazing-incidence small- and wide-angle X-ray scattering (GISAXS and GIWAXS) and X-ray fluorescence (XRF).

O 56.5 Wed 11:30 H4

Vortex Assisted Growth of Metallic Nanowires in Superfluid Helium Droplets — •Alexander Volk[1], Philipp Thaler[1], Andreas W. Hauser[1], Daniel Knez[2], Werner Grogger[2], Ferdinand Hofer[2], and Wolfgang E. Ernst[1] — [1]Institute of Experimental Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria — [2]Institute for Electron Microscopy and Nanoanalysis, TU Graz, Steyrergasse 17, 8010 Graz, Austria

Helium droplets provide an ideal matrix for the aggregation of tailored metallic nanoclusters and nanowires. The vortex guided growth process of the wires in the superfluid helium environment has not been fully understood yet. Silver represents a special case among the metals studied so far since no continuous wires were detected after surface deposition, which was attributed to some unexplained barrier formation by the helium. We have explored the growth process of silver nanowires in detail and show by high resolution transmission electron microscopy in combination with computer simulations under which conditions continuous nanowires are obtained. These insights enable us to deduce a model for the growth process of these wires inside the helium droplets from comparison of silver and gold nanowire morphologies. It shows further, that the morphologies of the nanowires can be controlled *via* the doping rates with which the metal atoms are added to the droplets during the synthesis process.

O 56.6 Wed 11:45 H4

Formation of Ag-Au core-shell clusters in superfluid helium nanodroplets studied by atomic resolution electron tomography — Philipp Thaler[1], Georg Haberfehlner[2], Alexander Volk[1], Gerald Kothleitner[2], and •Wolfgang E. Ernst[1] — [1]Institute of Experimental Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria — [2]Institute for Electron Microscopy and Nanoanalysis, TU Graz, Steyrergasse 17, 8010 Graz, Austria

Metallic nanoparticles consisting of a few thousand atoms are of large interest for potential applications in different fields such as optics, catalysis or magnetism. Structure, shape and composition are the basic parameters responsible for properties of such nanoscale materials. We report on the formation of metallic core-shell nanostructures in superfluid helium nanodroplets (He_N) and their subsequent surface deposition under soft landing conditions. Using atomic resolution electron tomography, we can clarify the structure and composition of our particles on an atomic level. This detailed analysis shines light on the growth process of the nanoparticles and will allow deliberate tuning between single core and multi-core structures in future experiments.

O 56.7 Wed 12:00 H4

Silver clusters in room temperature ionic liquids: supersonic nozzle expansion deposition — •Stefanie Roese, David Engemann, Andreas Gruhn, and Heinz Hövel — Fakultät Physik / DELTA, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

Promising stabilizers for nanoparticles are room temperature ionic liquids (RTIL), which are salts of weakly coordinating cations and anions being liquid at room temperature [1]. They consist of a large organic cation and a small inorganic anion. The different charges of the molecules cause a strong attractive interaction, while the large difference of size of the molecules prevents condensation at room temperature [2]. Due to their low vapor pressure RTIL can be used under vacuum conditions. BMIM PF6 is one of the most widely studied ionic liquids [3] and is here used for the generation and stabilization of silver nanoparticles.

The investigated silver nanoparticles are formed in a supersonic nozzle expansion [4] and deposited into the RTIL using a rotating cylinder for mixing. The cluster properties are investigated afterwards with UV/Vis absorption measurements, XANES and SAXS. The formation of a cation layer at the cluster surface could be observed.

[1] J. Dupont, J. D. Scholten, Chem. Soc. Rev. 39, 1780 (2010). [2] J. Dupont, Accounts of chemical research 44, 11 (2011). [3] P. Dash and R. W. J. Scott, Chem. Commun. 2009, 812. [4] H. Hövel, et al., Z. Phys. D 42, 203 (1997).

O 56.8 Wed 12:15 H4

The effect of different gas admixtures on nanoparticles formation in a gas aggregation source and their treatment by hollow cathode plasma — •Oleksandr Polonskyi, Amir Mohammad Ahadi, Thomas Strunskus, and Franz Faupel — Chair for Multicomponent Materials, Faculty of Engineering, Christian-Albrechts University at Kiel, Germany

Metal nanoparticles (NPs) have been of high scientific interest in the last decades as they have unique chemical, physical, electrical, magnetic and optical properties, which are particularly explored in combination with host matrix. Among the number of PVD methods for nanoparticles generation, the gas aggregation method has lately received an increased attention due to simplicity of NPs deposition and variety of parameters to control their properties (size, rate). The present talk is concerned with a such called Gas Aggregation cluster Source (GAS) for metal and metal oxide nanoparticles generation. New results of the influence of nanoparticles generation by admixing different gases into the GAS volume for noble metals (Ag, Cu) will be presented. The effect of helium/oxygen admixture on cluster formation is studied in detail. In addition we report on the combination of the established process of NPs generation by GAS with a hollow cathode (HC) plasma source for novel nanostructure formation. Here, an Ag nanoparticle beam has been treated by a HC plasma at different operation parameters.

O 57: Focus Session: Many-body effects in two-dimensional materials

Organizers: Christopher Gies and Tim Wehling (Universität Bremen)

Time: Wednesday 9:30–13:00 Location: H16

Invited Talk O 57.1 Wed 9:30 H16

Probing bandgap renormalization, excitonic effects, and interlayer coupling in 2D transition metal dichalcogenide semiconductors — •Miguel M. Ugeda[1], Aaron Bradley[1], Sufei Shi[1], Felipe H. Jornada[1], Yi Zhang[2,3], Diana Qiu[1], Wei Ruan[1], Sebastian Wickenburg[1], Alexander Riss[1], Jiong Lu[1], Sung-Kwan Mo[2], Zahid Hussain[2], Zhi-Xun Shen[3], Feng Wang[1], Steven G. Louie[1], and Michael F. Crommie[1] — [1]Department of Physics, University of California, Berkeley, CA 94720, USA. — [2]Advanced Light Source, Lawrence Berkeley National Lab., Berkeley, CA 94720, USA. — [3]Stanford Institute for Materials and Energy Sciences, Menlo Park, CA 94025, USA.

Reduced screening in 2D metal dichalcogenides (TMDs) has been predicted to result in dramatically enhanced Coulomb interactions that should cause giant bandgap renormalization and excitonic effects. Here we present direct experimental observation of extraordinarily high exciton binding energy and band structure renormalization in a single-layer of semiconducting TMD[1]. We have determined the binding energy of correlated electron-hole excitations in monolayer MoSe2 grown via molecular beam epitaxy on bilayer graphene by using a combination of scanning tunneling spectroscopy and photoluminescence spectroscopy. We have also studied the role of interlayer coupling and layer-dependent carrier screening on the electronic structure[2] of few layer MoSe2. We find that the electronic quasiparticle bandgap decreases by nearly 1 eV when going from one layer to three. [1]Nature Materials 13, 1091 (2014). [2]Nano Letters 15, 2594 (2015).

O 57.2 Wed 10:00 H16

A Tight Binding Approach to Strain and Curvature in Monolayer Transition-Metal Dichalcogenides — •Alexander Pearce and Guido Burkard — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

We present a model of the electronic properties of the monolayer transition-metal dichalcogenides based on a tight binding approach which includes the effects of strain and curvature of the crystal lattice. Mechanical deformations of the lattice offer a powerful route for tuning the electronic structure of the transition-metal dichalcogenides, as changes to bond lengths lead directly to corrections in the electronic Hamiltonian while curvature of the crystal lattice mixes the orbital structure of the electronic Bloch bands. We first present an effective low energy Hamiltonian describing the electronic properties near the K point in the Brillouin zone, then present the corrections to this Hamiltonian due to arbitrary mechanical deformations and curvature in a way which treats both effects on an equal footing. This analysis finds that local area variations of the lattice allow for tuning of the band gap and effective masses, where the application of uniaxial strain decreases the magnitude of the direct band gap at the K point. Additionally, strain induced bond length modifications create a fictitious gauge field but with a coupling that is smaller than seen in related materials like graphene. We also find curvature of the lattice leads to the appearance of both an effective in-plane magnetic field which couples to spin degrees of freedom and a Rashba-like spin-orbit coupling due to broken mirror inversion symmetry. (arXiv:1511.06254).

O 57.3 Wed 10:15 H16

Observation of charge density wave order in 1D mirror twin boundaries of single-layer MoSe2 — •Sara Barja[1], Sebastian Wickenburg[1], Zhen-Fei Liu[1], Yi Zhang[1], Hyejin Ryu[1], Miguel M. Ugeda[2], Zahid Hussain[1], Zhi-Xun Shen[3], Sung-Kwan Mo[1], Miquel B. Salmeron[1,2], Feng Wang[1,2], Michael F. Crommie[1,2], D. Frank Ogletree[1], Jeffrey B. Neaton[1,2], and Alexander Weber-Bargioni[1] — [1]Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [2]University of California at Berkeley, Berkeley, CA, USA — [3]Stanford Institute of Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA, USA

Detailed understanding of defect structure in 2D transition metal dichalcogenides may lead to control of the material properties. Here we provide direct evidence for the existence of isolated, 1D charge density waves (CDWs) at mirror twin boundaries (MTBs) in single-layer MoSe2. 4K-STM/STS measurements reveal a substantial bandgap of 60-140 meV opening at the Fermi level in the otherwise one dimensional metallic structure. We find an energy-dependent periodic modulation in the density of states along the MTB, with a wavelength of approximately three lattice constants. The modulations in the density of states above and below the Fermi level are spatially out of phase, consistent with CDW order. In addition to the electronic characterization, we determine the atomic structure and bonding configuration of the 1D MTB by means of high-resolution nc-AFM. DFT calculations reproduce both the gap opening and the modulations of the density of states.

O 57.4 Wed 10:30 H16

Probing the anisotropic interlayer Raman modes of few-layer ReS$_2$ — •Philipp Nagler, Gerd Plechinger, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040, Regensburg, Germany

ReS$_2$ has recently emerged as a new member in the rapidly expanding family of two-dimensional materials. Unlike MoS$_2$ or WSe$_2$, the optical and electrical properties of ReS_2 are not isotropic due to the reduced symmetry of the crystal. Here, we probe the anisotropic behavior of ReS_2 by Raman spectroscopy in the ultralow frequency regime. Thereby, we are able to access the layer breathing modes (LBM) and shear modes (LSM) of the material which stem from rigid-layer oscillations. The layer dependence of their peak positions enables an easy determination of the layer number of the crystal and can be readily reproduced by means of a monoatomic chain model. By varying the angle between the linearly polarized laser and the in-plane crystal axis, we are able to reveal an energetic shift of the LSM which is directly linked to the in-plane anisotropy of the shear modulus in this material.

30 min. Coffee Break

Invited Talk O 57.5 Wed 11:15 H16

Enhanced light-matter coupling and single-photon emission of atomically thin semiconductors — •Rudolf Bratschitsch — Westfälische Wilhelms-Universität Münster, Münster, Deutschland

Graphene is known as a prototypical two-dimensional material with unique physical properties. However, the difficulty of creating an optical band gap stimulated the search for other monolayer materials. In my talk I will show that atomically thin transition metal dichalcogenides serve as a promising new material class for opto-electronics and quantum optics [1-3]. In particular, I will explain, how gold nanoantennas may be used to increase the light-monolayer coupling and present single-photon emission from localized excitons in monolayer WSe2.

[1] P. Tonndorf et al., Optics Express 21, 4908 (2013)
[2] J. Kern et al., ACS Photonics 2, 1260 (2015)
[3] P. Tonndorf et al., Optica 2, 347 (2015)

Invited Talk O 57.6 Wed 11:45 H16

Optical Properties and Carrier Dynamics in Transition Metal Dichalcogenides — •Alexander Steinhoff-List[1], Malte Rösner[1,2], Matthias Florian[1], Michael Lorke[1], Christopher Gies[1], Ji-Hee Kim[3], Deok-Soo Kim[4], Chanwoo Lee[4], Gang Hee Han[3], Mun Seok Jeong[3,4], Tim Wehling[1,2], and Frank Jahnke[1] — [1]Institut für Theoretische Physik, Universität Bremen, P.O. Box 330 440, 28334 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, 28334 Bremen, Germany — [3]Center for Integrated Nanostructure Physics, Institute for Basic Science, Suwon 440-746, Republic of Korea — [4]Department of Energy Science, Sungkyunkwan University, Suwon 440-746, Republic of Korea

As two-dimensional transition metal dichalcogenides are promising candidates for optoelectronic applications, there is a strong interest in understanding the influence of excited carriers in these materials on optical properties. We present studies of absorption and photoluminescence spectra of monolayer MoS_2 in the presence of excited carriers as well as carrier kinetics, based on material-realistic ab-initio band structures and interaction matrix elements. It is shown that absorption spectra are strongly modified due to band-gap renormalization and screening effects, while the photoluminescence signal can be distinctly influenced by optical excitation above or below the electronic band gap. Moreover, we present results for carrier-carrier Coulomb and carrier-phonon scattering after optical excitation of the monolayer, exhibiting ultra-fast carrier relaxation on the sub-100 fs time scale.

O 57.7 Wed 12:15 H16

Microscopic modeling of the homogeneous linewidth in absorption spectra of TMDs — •Malte Selig[1], Gunnar Berghäuser[2], Ermin Malic[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

Monolayer transition metal dichalcogenides (TMDs) are direct-gap semiconductors with strong light-matter and Coulomb interaction. The latter accounts for strongly bound excitons, which dominate the optical spectrum. Here, we investigate the homogeneous linewidth in excitonic spectra induced by radiative coupling and exciton-phonon scattering. In conventional semiconductors, the radiative dephasing / recombination is typically weak in comparison to the electron-phonon scattering which mainly determines the homogeneous linewidth. The situation turns out to be different in atomically thin TMDs. Based on the density matrix formalism combined with the tight-binding approximation, we explicitly calculate the dephasing rates stemming from exciton-radiation interaction and exciton-phonon scattering. We find that in TMDs the radiative coupling is in the range of 1 meV clearly exceeding the exciton-phonon rate. We systematically investigate the resulting homogenous linewidth in absorption spectra of the most prominent TMDs for different temperatures, dopings, and substrates. [1]

[1] Galan Moody et al. Nat Commun 6, 8315 (2015)

O 57.8 Wed 12:30 H16

Influence of the spin-orbit splitting on the coupled spin-valley-dynamics in monolayer transition metal dichalcogenides — •Gerd Plechinger, Philipp Nagler, Sven Gelfert, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

Single layers of transition metal dichalcogenides (TMDCs) like MoS_2 and WS_2 can be produced by simple mechanical exfoliation. Offering a direct bandgap at the K-points in the Brillouin zone, they represent promising semiconductor materials for flexible and transparent optoelectronic applications. Due to inversion symmetry breaking together with strong spin-orbit-interaction, the valley and spin degrees of freedom are coupled in monolayer TMDCs. Via circularly polarized optical excitation, an efficient polarization of the K^+ or the K^- valley can be generated. Here, we investigate the dynamics of these coupled spin-valley polarizations in monolayer MoS_2 and WS_2 by means of photoluminescence spectroscopy and time-resolved Kerr rotation (TRKR). The results indicate a maximum achievable spin-valley-lifetime in these materials exceeding one nanosecond at low temperatures. Furthermore, we extract the dependence of the spin-valley lifetime on temperature. By varying the excitation energy, we reveal the excitonic resonances as well as the spin-polarized bandstructure around the K valleys common to monolayer TMDCs.

O 57.9 Wed 12:45 H16

Ultrafast Coulomb-induced intervalley coupling in atomically thin WS_2 — Robert Schmidt[1], •Gunnar Berghäuser[2], Malte Selig[3], Philipp Tonndorf[1], Ermin Malic[2], Andreas Knorr[3], Steffen Michaelis de Vasconcellos[1], and Rudolf Bratschitsch[1] — [1]Institute of Physics and Center for Nanotechnology, University of Münser, Münster Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden — [3]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Monolayers of semiconducting transition metal dichalcogenides hold the promise for a new paradigm in electronics by exploiting the valley degree of freedom in addition to charge and spin. For these materials valley polarization can be conveniently initialized and read out by circularly polarized light. However, the underlying microscopic processes governing the valley polarization in these atomically thin equivalents of graphene are still not fully understood. Here, we present a theoretical study on the ultrafast time-resolved intervalley dynamics in monolayer WS_2 [1]. Based on a microscopic theory, we reveal the many-particle mechanisms behind the observed spectral features. We show that Coulomb-induced intervalley coupling explains the immediate and prominent pump-probe signal in the unpumped valley as well as the seemingly low valley polarization degrees typically observed in pump-probe measurements if compared to photoluminescence studies.

[1] R. Schmidt et al, submitted (2015)

O 58: Organic-Inorganic Systems III: Metal-Organics

Time: Wednesday 15:00–18:00 Location: S054

O 58.1 Wed 15:00 S054

Oxidation State Tuning in Ligand-Metal Surface Reaction: Formation of M(III)-Corroles on Ag(111) — •Malte Zugermeier[1], Nicolas Bock[1], Min Chen[1], Falk Niefind[1], Jan Herritsch[1], Lukas Ruppenthal[1], Martin Schmid[1], Peter Schweyen[2], Martin Bröring[2], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Germany

Surface-supported planar metal complexes are of high technical interest for catalytic applications combining the advantages of heterogeneous and homogeneous catalysis. However, a high degree of control over the chemical and electronic properties of the metal centers is required. While this control can be achieved by the attachment of axial ligands, these ligands compete with the reactants for the axial coordination site. Therefore, a more suitable solution is achieved by modification of the planar ligand. We demonstrate that adsorbed corroles on Ag(111) oxidize metal atoms to their +III state and form the corresponding metal complexes. In contrast, adsorbed porphyrins and phthalocyanines can oxidize co-adsorbed metal atoms only to +II ions. Corroles differ from the closely related porphyrins by the absence of a single carbon atom in the macrocycle. The resulting size-reduced ring provides a tighter coordination environment and stabilizes higher oxidation states. Specifically, we studied monolayers and multilayers of an octa-alkyl corrole and their reaction with Ni and Co atoms on a Ag(111) surface by XPS, UPS and STM.

O 58.2 Wed 15:15 S054

Molecular adsorption and self-assembled structures of tetra(cyanophenyl)porphyrin on Cu(111) and ultrathin CoO as substrate — •Tobias Schmitt, Marco Raschmann, Lutz Hammer, and M.Alexander Schneider — Solid State Physics, University Erlangen-Nürnberg, 91058 Erlangen, Germany

Molecular self-assembly on surfaces is controlled by a complex balance between molecule-substrate and intermolecular interactions. We report on the adsorption geometry of single molecules and ordered phases of free-base meso-tetra(m-cyanophenyl)porphyrin (TCNPP) on Cu(111) and on CoO(111)/Ir(100) thin films using low-temperature scanning tunneling microscopy in ultrahigh vacuum. The molecules were deposited at different substrate temperatures to activate diffusion and potential self-assembly processes. When depositing TCNPP onto the Cu(111) surface at T=293K intermolecular H-bonding and dipolar coupling are found to be the dominating inter-molecular interactions but extended ordered structures are not formed. Already at slightly higher temperatures 2-fold metal-ligand coordination comes into play and starts dominating the assembly of linear structures on Cu(111). The molecules themselves remain unmetalated. Also on thin CoO(111) films TCNPP molecules cluster into islands with little tendency to form ordered structures when adsorbed at T=293K . When heated to T=420K the TCNPPs surprisingly show a different internal structure in STM images akin to metalated molecules. At this temperature also networks are observed that show a 3- or 4-fold coordination which we interpret as a sign of metal coordination at the CoO surface.

O 58.3 Wed 15:30 S054

Intermolecular interactions among TiOPc molecules on Ag(111) — •Laura Fernández[1], Sebastian Thussing[1], Antón Brión-Ríos[2], Pepa Cabrera-San Felix[2], Daniel Sánchez-Portal[3], and Peter Jakob[1] — [1]Fachbereich Physik, Philipps- Universität Marburg, Renthof 5, 35032 Marburg, Germany — [2]DIPC, Paseo Manuel Lardizábal 4, 20018 San Sebastián, Spain — [3]Centro de Física de Materiales CSIC-UPV/EHU. Paseo Manuel Lardizábal 5, 20018 San Sebastian, Spain

The structure and intermolecular interactions of TiOPc deposited on Ag(111) has been investigated by IR spectroscopy and SPA-LEED. Additionally, the structure and bonding strength of the TiOPc/Ag(111) system has been explored by DFT. According to IR data, deposition of TiOPc (sub)monolayers leads to a “TiO-up” adsorption geometry of the molecules on Ag(111). Moreover, we find unambiguous evidence for an attractive interaction between neighboring TiOPc molecules, which leads to the formation of 2D islands with well-defined long range order (c-phase) upon cooling (sub)monolayer films to temperatures below 70K. This behavior is ascribed to the dominance of van der Waals interactions between adsorbed TiOPc molecules, and it is in contrast to the intermolecular repulsion observed for the CuPc/Ag(111) system. Repulsive intermolecular interactions induced by the parallel oriented dipoles of the TiO groups are negligible presumably due to the large lateral molecular dimensions. According to DFT calculations, the molecule-metal interaction of TiOPc on Ag(111) is notably weaker than in the case of CuPc, and it is lacking any net charge transfer.

O 58.4 Wed 15:45 S054

A new perspective on the adsorption behavior of nonplanar phthalocyanines on Cu(111) — •Elisabeth Wruss[1], Shashank S. Harivyasi[1], David A. Egger[2], Oliver T. Hofmann[1], Elisabeth Verwuester[1], Alexander Gerlach[3], Nahid Ilyas[4], Frank Schreiber[3], Oliver L. A. Monti[4], and Egbert Zojer[1] — [1]Graz University of Technology, Graz, Austria. — [2]Weizmann Institute of Science, Rehovoth, Israel. — [3]Universität Tübingen, Tübingen, Germany — [4]University of Arizona, Tucson, USA

The geometric and electronic properties of nonplanar, chlorinated members of the phthalocyanine family, namely chlorogallium phthalocyanine and chloroboron subphthalocyanine upon adsorption on Cu(111) are investigated, using DFT simulations including the vdW-surf correction. The comparison with experimental results including x-ray standing wave, ultraviolet photoelectron spectroscopy and scanning tunneling microscopy yields strong indications of a dissociation of the molecules upon adsorption associated with a loss of the Cl atom as one possible scenario. For the chlorogallium phthalocyanine system, the experimental and calculated adsorption heights and adsorption-induced work-function shifts yield good quantitative agreement. Surprisingly, the same work-function change is also found for the adsorption of intact ”Cl-down” molecules, despite hugely different geometries and molecular dipoles. This seeming contradiction can be explained as a consequence of Fermi-level pinning. Our findings show that the adsorption process of chlorinated phthalocyanines and related molecules is considerably more complex than previously assumed.

Invited Talk O 58.5 Wed 16:00 S054

Thin Films of Metal-Organic Frameworks: Functional, photoswitchable coatings and unique model systems — •Lars Heinke — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Deutschland

Metal-organic frameworks (MOFs) are nanoporous, crystalline materials, assembled from metal notes and organic linker molecules. In addition to many potential applications of the (conventional) powder MOF material, well-defined thin films seem perfectly suited for challenging uses and as unique model systems, where certain molecular and MOF properties can be precisely measured by applying surface sensitive techniques. These thin films are prepared in a layer-by-layer fashion on a solid substrate by using liquid-phase epitaxy, referred to as the SURMOF-approach.

Incorporating photochromic molecules like azobenzene in the crystalline structure enables the switching of physical and chemical MOF properties by light. This can be used for various uses, such as realizing the remote-controlled release of guest molecules from a nanoporous container.

These thin films also enable detailed investigations of the molecules which are incorporated in the crystalline structure, unlike investigating these molecules in solution. In this way, the isomerization of isolated azobenzene moieties could be investigated.

Recently, the electronic structure and electrical properties of MOFs have become a research focus. SURMOFs have been used to investigate the direction-dependent conductivity in anisotropic MOF structures.

O 58.6 Wed 16:30 S054

Tetrapyrrole metalation with rare earths — •Katharina Diller[1], Aparajita Singha[1], Christian Wäckerlin[1], Jan Dreiser[2], Alberto Verdini[3], Albano Cossaro[3], Luca Floreano[3], and Harald Brune[1] — [1]École Polytechnique Fédérale de Lausanne, Switzerland — [2]Paul Scherrer Institute, Switzerland — [3]CNR-IOM, Laboratorio Nazionale TASC, I-34149 Trieste, Italy

The *in vacuo* metalation of tetrapyrrole molecules is a convenient way to build tetrapyrrole-based metal-organic structures on metal surfaces.

A commonly employed route is the deposition of molecules by organic molecular beam epitaxy, which subsequently are exposed to a beam of metal atoms. Given the importance of terbium phthalocyanine double decker compounds as single molecule magnets, it is surprising that so far on-surface metalation predominantly focused on the creation of transition metal complexes, with only few scanning tunneling microscopy (STM) studies dedicated to the rare earth Ce [1, 2]. Here, we follow the metalation of free-base tetraphenylporphyrin and free-base phthalocyanine molecules on Ag(111) with different rare earth metals using a combination of scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and near-edge X-ray absorption fine-structure (NEXAFS) spectroscopy. We show that metalation can be readily achieved at room temperature, and discuss the effects of an excess of metal atoms on the spectroscopic signatures.

[1] D. Écija et al., Angew. Chem. Int. Ed., 2011, 50, 3872, [2] A. Weber-Bargioni et al., J. Phys. Chem. C, 2008, 112, 3453.

O 58.7 Wed 16:45 S054

Electric transport properties of pristine and loaded surface-anchored metal-organic frameworks — Jianxi Liu[1], Tobias Wächter[2], Andreas Irmler[3], Peter G. Weidler[1], Hartmut Gliemann[1], Fabian Pauly[3], Veronica Mugnaini[1], •Michael Zharnikov[2], and Christof Wöll[1] — [1]Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Applied Physical Chemistry, University of Heidelberg, 69120 Heidelberg, Germany — [3]Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Understanding of the electric transport through surface-anchored metal-organic frameworks (SURMOFs) is important both from a fundamental perspective as well as with regards to possible future applications in electronic devices. To address this mostly unexplored subject, we integrated a series of representative SURMOF thin films, formed by copper nodes and trimesic acid and known as HKUST-1, in a mercury-drop based tunneling junction. Although the transport properties of these SURMOFs are analogous to those of hybrid metal-organic molecular wires, manifested by a very low value of the tunneling decay constant ($\beta = 0.006\ 1/\text{Å}$), they are at the same time found to be consistent with a linear increase of resistance with film thickness. Upon loading of SURMOF pores with ferrocene or tetracyanoquinodimethane (TCNQ), a noticeable increase in transport current was observed, being especially dramatic (6 orders of the magnitude) in the case of TCNQ. Relevant structural and transport models are discussed.

O 58.8 Wed 17:00 S054

Synthesis of Organometallic Sandwich Complexes and Nanowires on Graphene — •Felix Huttmann, Nicolas Schleheck, Merve Seçkin, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

Organometallic sandwich-molecular nanowires of europium-cyclooctatetraene (EuCot) and vanadium-benzene (VBz) have been theoretically predicted to have interesting electronic structures: Semiconducting and ferromagnetic (EuCot) [1] or half-metallic and ferromagnetic with full spin polarization of the conduction band (VBz) [2]. They thus have potential for efficient spin filters. Here, we have pursued their growth from the constituent vapors on an inert graphene surface, and investigated the samples *in situ* using scanning tunneling microscopy. EuCot nanowires form readily, and by varying the growth conditions, we find a rich spectrum of morphologies, from a disordered, spaghetti-like growth to highly ordered, anisotropically shaped, two-dimensional crystallites made of wire bundles. In these bundles, the wires are offset against their nearest neighbors to allow the wires to hook into each other, and where wire bundles bend, a characteristic bending angle is often observed to accommodate this. In contrast, for VBz only sandwich molecules of composition VBz$_2$ could be produced, but no wires. VBz$_2$ molecules form overlayers and desorb at around room temperature.

[1] Ke Xu et al., J. Chem. Phys. 131, 104704 (2009)

[2] V. V. Maslyuk et al., Phys. Rev. Lett. 97, 097201 (2006)

O 58.9 Wed 17:15 S054

Metalation of porphyrin with Mg on Ag(100) — •Gianluca Di Filippo, Andrej Classen, Rebecca Pöschel, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058, Erlangen, Germany

Porphyrins are a class of π-conjugated organic molecules of high technological interest. Their optical, electronic and chemical properties make them very suitable for energy production in solar cells, phototherapy, and catalysis [1]. Porphyrins are composed of a macrocycle of four pyrrole rings (C_4H_4N-) connected by methine units ($=CH-$). The nitrogen atoms at the interior form a central pocket ideal to incorporate metal atoms and to obtain metal-porphyrins by direct metalation of molecules adsorbed on inert metal surfaces [2].

Using X-Ray photoelectron spectroscopy (XPS) we investigated the in situ metalation of one monolayer tetraphenylporphyrin (2HTPP) on Ag(100) with Mg atoms. This reaction results in the formation of adsorbed magnesium(II)-tetraphenylporphyrin (MgTPP). The metalation is observed to take place either by evaporating Mg atoms on top of the 2HTPP monolayer or by depositing 2HTPP on top of the Ag surface with adsorbed Mg atoms. In the second case, the presence of oxygen contamination and consequent MgO formation reduces the efficiency at which Mg atoms are embedded in the molecule macrocycle.

[1] W. Auwärter *et al.*, Nature Chemistry, **7**, 105 (2015)

[2] J.M. Gottfried *et al.*, J. Am. Chem. Soc., **128**, 5644 (2006) - F. Buchner *et al.*, J. Phys. Chem. C, **112**, 15458 (2008)

O 58.10 Wed 17:30 S054

Metalation of porphyrins on metal and oxide surfaces — •Ole Lytken, Michael Röckert, Matthias Franke, Daniel Wechsler, Quratulain Tariq, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg

Porphyrins are large conjugated organic molecules with four pyrrole units capable of coordinating either two protons or a metal ion in the center of the molecule. Both metalated and unmetalated molecules can be deposited on surfaces under ultrahigh vacuum using physical vapor deposition. However, once deposited the unmetalated molecules might react with the substrate they have been deposited on and metalate. We have studied this self-metalation reaction of 5,10,15,20-tetraphenylpoprhyrin (2HTPP) on Cu(111), a metal surface, and MgO(100), an oxide surface. On both surfaces the reaction with the substrate occurs at, or slightly above, room temperature, forming CuTPP and MgTPP, respectively. The project is supported by the DFG through FOR 1878 (funCOS).

O 58.11 Wed 17:45 S054

Surface-assisted reactions of porphyrins investigated by nc-AFM — •Jacob Ducke, Yuanqin He, Felix Bischoff, Manuela Garnica, and Willi Au — TU München, Germany

Surface-assisted covalent linking of precursor molecules enables the fabrication of low-dimensional nanostructures. Here, we present a temperature-induced covalent dehydrogenative coupling mechanism of free-base porphine (2H-P) units. The oligomers resulting from a homocoupling reaction have been characterized by a multitechnique approach and theoretical modelling, however an atomically resolved study of the resulting nanostructures was lacking [1]. With nc-AFM we are able to identify the resulting bonding motifs and can confirm the proposed structural models. Furthermore, we used a similar coupling mechanism to functionalize the edges of epitaxial grown graphene on Ag(111) with 2H-P [2]. Distinct configurations are identified and resolved at the graphene edges with submolecular precision. Functionalization reactions like metallation of the 2H-P and subsequent axial ligation of adducts are conserved for porphines coupled to graphene. Thus, our findings bear promise for functionalized graphene nanostructures and for the formation of tailored oligomeres on surfaces.

[1] Wiengarten, A., et al. "Surface-assisted dehydrogenative homocoupling of porphine molecules." J. Amer. Chem. Soc. 136 (2014): 9346-9354.

[2] He, Y., et al. "Fusing tetrapyrroles to graphene edges by surface-assisted covalent coupling." submitted

O 59: Photonics and Nanooptics III: Fabrication and Characterization

Time: Wednesday 15:00–18:15 Location: S051

O 59.1 Wed 15:00 S051

Magnesium for Active Plasmonics in the Visible Wavelength Range — •Florian Sterl, Nikolai Strohfeldt, Ramon Walter, Andreas Tittl, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Investigating new materials plays an important role for advancing the field of nanoplasmonics. Here we fabricate nanodisks from magnesium and demonstrate tuning of their plasmon resonance throughout the whole visible wavelength range by changing the disk diameter. Furthermore, we employ a catalytic palladium cap layer to transform the metallic Mg nanoparticles into dielectric magnesium hydride nanoparticles when exposed to hydrogen gas. We prove that this transition can be reversed in the presence of oxygen. The addition of a titanium buffer layer which separates the Mg and Pd layers from each other significantly enhances the (un)loading dynamics of the particles. During the transition from Mg to MgH_2, the plasmon resonance disappears within minutes. When the particles are dehydrogenated, the resonance is fully restored in 10-20 minutes. Large-area samples covered with such nanodisks thus feature an extinction peak that can be repeatedly switched on and off or kept at any intermediate state, which offers new perspectives for active plasmonic metamaterials. Our findings can also contribute to a better understanding of the H_2 diffusion dynamics in Mg, which can lead to new insights for H_2 storage applications. To this end, we use dark field spectroscopy to observe the scattering spectrum of single Mg nanocrystals during (de)hydrogenation, and make first steps to reproduce our observations in numerical simulations.

O 59.2 Wed 15:15 S051

Thermodynamics of Hydrogen in Palladium Nanoparticles — •Nikolai Strohfeldt[1], Ronald Griessen[2], and Harald Giessen[1] — [1]4. Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Faculty of Sciences, Division of Physics and Astronomy, VU University, Amsterdam, The Netherlands

Palladium-hydrogen is a prototypical metal-hydrogen system, which is well suited for active plasmonics. Upon hydrogenation of Pd to PdH_x, the dielectric function and particle size changes quite severely. These changes can be traced through the plasmonic resonance, in situ, which enables us to optically study microscopic changes in our system. Recently, a lot of attention has been devoted to the ab- and desorption of hydrogen in nanosized plasmonic palladium particles. Here, we show that the large body of data on the thermodynamics of palladium nanostructures available so far in literature exhibits general patterns that lead to unambiguous conclusions about the detailed microscopic processes involved in H absorption and desorption in Pd nanoparticles that can be used as prototypes for active plasmonic elements. On the basis of a remarkably robust scaling law for the hysteresis in absorption-desorption isotherms, we also show that hydrogen absorption in palladium nanoparticles is consistent with a coherent interface model and is thus clearly different from bulk Pd behaviour. However, H desorption occurs fully coherently only for small nanoparticles at temperatures sufficiently close to the critical temperature. For larger particles it is partially incoherent as in bulk, where dilute α-PdH_x and high concentration β-PdH_x phases coexist.

O 59.3 Wed 15:30 S051

Simple, but complicated surface chemistry for Surface Plasmon resonance sensor — Thidarat Wangkam[1], •Toemsak Srikhirin[2], Boonsong Sutapun[3], Kawin Nawattanapaiboon[2], Supaporn Kanjai[1], Armote Somboonkaew[4], and Rathasart Amarit[4] — [1]Department of Industrial Physics and Medical Instrumentation, Faculty of Applied Science, King Mongkut*s University of Technology North Bangkok, Thailand — [2]Materials Science and Engineering Programme, Faculty of Science, Mahidol University, Bangkok — [3]School of Electronics Engineering, Suranaree University of Technology, Thailand — [4]Photonics Technology Laboratory,National Electronics and Computer Technology Center,Thailand

Thin metal planar surface would bring us to the fascinated plasmon resonance phenomena. This characteristic is specified some optical properties on the surface under a penetration depth about 200-300 nm on the metal surface. Surface plasmons resonance sensor has been employed in a wide spectrum of studies ranging from biosensor, electrochemistry, thin film, surface plasmon microscopy and nanoparticles. This work would be shown a variety of surface chemistry which were performed on the surface Plasmon sensor. Multiplexed of gold nanoparticle and magnetic nanoparticle were combined with a variety of biological samples (Protein chip, allergy, biomarkers etc.) for real-time detection on SPR spectroscopy. Moreover, the SPR sensor chip has been designed with simple platform for a complicated body fluids samples for clinical diagnostic further.

O 59.4 Wed 15:45 S051

Bottom-up synthesis of large area single-crystalline atomically flat gold flakes with single-crystalline silver cubes as single quantum emitter nanoantennas — •Simon Ristok, Bettina Frank, and Harald Giessen — University of Stuttgart, 4th Physics Institute and Research Center SCoPE, Pfaffenwaldring 57, 70569 Stuttgart, Germany

When using quantum emitters such as NV centers in diamond, quantum dots, or dye molecules as effective photon sources, it is often necessary to control certain characteristics of the emitted radiation, i.e., the emission rate and direction. A promising approach is the coupling of the emitters to a plasmonic nanoantenna. In this work, we fabricate plasmonic nanopatch antennas using exclusively bottom-up methods. The antennas consist of silver nanocubes which are positioned over the atomically flat surface of a gold microplatelet. Both Ag nanocubes and Au microplatelets are single-crystalline and are separated by a dielectric polymer spacer layer. The plasmonic resonance of the antennas can be tuned by varying the size of the Ag nanocubes and the thickness of the nm-thick spacer layer. The further steps include the embedding of fluorescent dye molecules into the gap of the nanopatch antenna, followed by fluorescence enhancement and lifetime measurements. Investigating this system can help us understand the prerequisites to expand the range of emitters also to NV centers and quantum dots.

O 59.5 Wed 16:00 S051

Helium-Ion Milling of Gold Nanoantennas: Toward Plasmonics with Nanometer Precision — •André Beyer[1], Henning Vieker[1], Heiko Kollmann[2], Xianji Piao[3], Namkyoo Park[3], Martin Silies[2], Christoph Lienau[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems and Surfaces, Bielefeld University, 33615 Bielefeld — [2]Institute of Physics and Center of Interface Science, Carl von Ossietzky University Oldenburg, 26129 Oldenburg — [3]Photonic Systems Laboratory, School of Electrical Engineering, Seoul National University, 151-742 Seoul, Korea

Plasmonic nanoantennas are versatile tools for coherently controlling and directing light on the nanoscale. For these antennas, current fabrication techniques such as electron beam lithography (EBL) or focused ion beam (FIB) milling with Ga^+-ions routinely achieve feature sizes in the 10 nm range. However, they suffer increasingly from inherent limitations when a precision of single nanometers down to atomic length scales is required, where exciting quantum mechanical effects are expected to affect the nanoantenna optics. Here, we demonstrate that a combined approach of Ga^+-FIB and milling-based He^+-ion lithography (HIL) for the fabrication of nanoantennas offers to readily overcome some of these limitations. Gold bowtie antennas with 6 nm gap size were fabricated with single-nanometer accuracy and high reproducibility. Using third harmonic (TH) spectroscopy, we find a substantial enhancement of the nonlinear emission intensity of single HIL-antennas compared to those produced by state-of-the-art gallium-based milling.

O 59.6 Wed 16:15 S051

Long-range plasmon coupling in self-assembled colloidal monolayers — •Joseph P.S. Fitzgerald, Kirsten Volk, Tobias Honold, and Matthias Karg — Physical Chemistry I, University of Bayreuth, Germany

Localized surface plasmon resonances (LSPRs) of metal nanoparticles show large interaction cross sections with incident light and intense surface near-fields, but with large optical losses and short coherence times. Two-dimensional lattices of plasmonic particles can support high Q-factor collective resonances, with increased intensity, reduced losses, and increased excitation lifetimes. Here, we report on the plasmonic properties of highly-ordered monolayers of metal-hydrogel core-shell particles prepared using an interfacial self-assembly protocol [1].

This method allowed us to produce hexagonal lattices with a range of interparticle spacings 350-550 nm [2]. We found that the resonance peak position, intensity, and width depend strongly on the interparticle spacing. We show that this is due to long-range dipole-dipole coupling between individual nanoparticles using the coupled dipole approximation (CDA). The results are further supported by finite-difference time-domain (FDTD) calculations, allowing detailed analysis of lattice near-fields. The presented approach is an important step toward higher Q-factor plasmonic materials for several nano-optical applications.

[1] T. Honold, K. Volk, A. Rauh, J.P.S. Fitzgerald, M. Karg. J. Mater. Chem. 3 (2015) 11449-11457.

[2] K. Volk, J.P.S. Fitzgerald, M. Retsch, M. Karg. Adv. Mater. (2015).

O 59.7 Wed 16:30 S051

Efficient Surface Plasmon Excitation via Inelastic Electron Tunneling — •Eric Jehnes and Lukas M. Eng — Institut für Angewandte Physik, TU Dresden, Deutschland

Surface plasmon polaritons (SPPs) can be described as electromagnetic waves that are localized at metal-dielectric interfaces. Such surface-bound fields are caused by electron-density oscillations that may be excited by both photons and electrons. While current research mostly focuses on light-excited SPPs, the interaction with charged particles such as electrons is often neglected.

This contribution concentrates on the excitation of SPPs via inelastic electron tunneling in metal-insulator-metal and metal-insulator-semiconductor junctions. Such tunneling junctions emit visible light [1] of a specific wavelength and polarization, clearly depending on the nanoscopic structure of the metal electrode. Far-field imaging and spectroscopic measurements were used to characterize the fabricated samples. The conversion from electrical to optical signal is limited only by the tunneling time itself and enables high bandwidths, which is of relevance for telecommunication and optical interconnect applications. With current lithographic techniques at hand, nanoscopic light emitting tunneling junctions can easily be integrated into opto-electronic devices.

[1] J. Lambe and S. L. McCarthy, Phys. Rev. Lett. 37, 923 (1976)

O 59.8 Wed 16:45 S051

Plasmonic Coupling in Core/Satellite Nanoclusters — •Christian Kuttner[1,2], Roland Höller[1,2], Martin Dulle[3], Sabrina Thomä[2], Martin Mayer[1], Stephan Förster[3], Andreas Fery[1,2], and Munish Chanana[2,4] — [1]Nanostructured Materials, Leibniz Institute of Polymer Research, 01069 Dresden, Germany — [2]Physical Chemistry II, University of Bayreuth, 95440 Bayreuth, Germany — [3]Physical Chemistry I, University of Bayreuth — [4]Institute of Building Materials, ETH Zürich, 8093, Zürich, Switzerland

We present the fundamental coupling scenarios in core/satellite nanoclusters prepared from colloidal assembly of small spherical gold or silver NPs (as satellites) onto larger gold NPs (as cores). The resulting dispersions exhibit high colloidal stability and allowed for the precise characterization of the core/satellite architecture in dispersion by small-angle X-ray scattering (SAXS).

Strong near-field coupling between the building blocks results in distinct regimes of dominant satellite-to-satellite and core-to-satellite coupling. High robustness against satellite disorder was proved by UV/Vis diffuse reflectance (integrating sphere) measurements. Generalized multi particle Mie theory (GMMT) simulations were employed to describe the electromagnetic coupling within the nanoassemblies.

Roland P. M. Höller *et al.*, **2015** (submitted).

O 59.9 Wed 17:00 S051

Improved anodisation of aluminium thin films through reactive sputtering — •Fabian Patrovsky[1], Vera Fiehler[1], Susan Derenko[1], Matthias Böhm[1], Stephan Barth[2], Hagen Bartzsch[2], Peter Frach[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Physik, TU Dresden, Deutschland — [2]Fraunhofer-Institut für Organische Elektronik, Elektronenstrahl- und Plasmatechnik FEP, Dresden, Deutschland

Anodised aluminium oxide (AAO) templates are widely used to fabricate plasmonic nanorod and nanowire arrays as well as sophisticated meta-materials [1]. However, manufacturing those structures on a substrate has always proven to be very difficult; either an elaborate membrane transfer is necessary [2] or previously deposited aluminium layers (CVD or PVD) have to be anodised directly, which often leads to poor results [3].

In this study we present a method which greatly improves anodisation of sputtered aluminium thin films. By introducing oxygen into the sputtering plasma, we create a highly amorphous aluminium layer that exhibits a very low defect density after anodisation, while yielding highly reproducible results. This approach enables us to reliably fabricate plasmonic nanorod arrays with improved optical properties.

[1] A. Eftekhari, Nanostructured Materials, Wiley-VHC, (2008)

[2] Z. Zhan and Y. Lei, ACS Nano 8, 3862 (2014)

[3] M. Es-Souni and S. Habouti, Frontiers in Metamaterials 1 (19), (2014)

O 59.10 Wed 17:15 S051

Seed-Mediated Growth of Bimetallic Plasmonic Nanostructures and their Use for Chemical Reaction Sensing — •Domenico Paone, Nikolai Strohfeldt, Florian Sterl, and Harald Giessen — 4th Physics Institute and Research Center SCOPE, University of Stuttgart

Plasmonic nanostructures show unique optical properties by focusing down light into the sub-wavelength scale. These properties can be used in several practical applications like e.g. gas or chemical sensing. The resonance behavior of such nanoparticles is strongly size and shape dependent. Therefore, it is essential to develop methods for growing nanostructures in various geometries at high yield and low costs. In this work, we present a seed-mediated growth method for gold nanorods that enables the variation of the rodlength using CTAB-capping. We characterize these nanorods optically with ensemble UV-Vis spectroscopy. To study the properties and quality of individual nanorods, we also employ single-particle dark-field spectroscopy. Furthermore, we synthesize Pd overcoated Au nanorods to investigate optically the hydrogen diffusion into extremely small, but well defined palladium structures. We find pronounced spectral shifts upon exposure to different hydrogen concentrations.

O 59.11 Wed 17:30 S051

Controlled Living Nanowire Growth: Precise Control over the Morphology and Optical Properties of AgAuAg Nanowires — •Martin Mayer[1], Leonardo Scarabelli[2], Katia March[3], Thomas Altantzis[4], Moritz Tebbe[5], Mathieu Kociak[3], Sara Bals[4], F. Javier García de Abajo[6], Luis M. Liz-Marzán[2], and Andreas Fery[1] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]CIC biomaGUNE, Donostia, Spain — [3]Laboratoire de Physique des Solides, University Paris-Sud, Orsay, France — [4]EMAT, University of Antwerp, Antwerp, Belgium — [5]Physical Chemistry II, University of Bayreuth, Bayreuth, Germany — [6]Institut de Ciencies Fotoniques, Barcelona, Spain

Inspired by the concept of living polymerization reaction, we are able to produce bimetallic noble metal nanowires with a precise control over their morphology and plasmonic properties. By establishing a constant silver deposition rate on the tips of pentatwinned gold nanorods used as seed cores, the lengths of the AgAuAg nanowires increases linearly in time with nanometer control.

Due to the extraordinary low polydispersity of the resulting nanowires, plasmonic modes up to the 8th order can clearly distinguished in UV–vis/NIR spectroscopy of colloidal solutions.

We analyze the spatial distribution and the nature of the plasmons on the single nanowire level by electron energy loss spectroscopy and obtain excellent agreement between measurements and electromagnetic simulations. This procedure opens up new possibilities for the exploitation of plasmon resonances in the near and mid IR regions.

O 59.12 Wed 17:45 S051

Complete analysis of plasmon transmission through top-down fabricated monocrystalline nanowires — •Enno Krauss[1], Gary Razinskas[1], Peter Geisler[1], and Bert Hecht[1,2] — [1]NanoOptics & Biophotonics Group, Experimentelle Physik 5, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Röntgen Research Center for Complex Material Systems (RCCM), Am Hubland, 97074 Würzburg, Germany

Exact quantitative understanding of plasmon propagation along nanowires is mandatory for designing and creating functional devices. We investigate plasmon transmission through top-down fabricated single crystalline gold nanowires on a glass substrate. We show that the transmission through finite length nanowires can be described by Fabry-Pérot oscillations that beat with free-space propagating light launched at the incoupling end. Using this extended Fabry-Pérot model, experimental and simulated length dependent transmissions agree quantitatively with a fully analytical model.

O 59.13 Wed 18:00 S051

3D chiral metamaterials made by direct laser writing — •Ioanna Sakellari[1], Xinghui Yin[1], Maxim Nesterov[1], Andre Radke[1], Konstantina Terzaki[2], Aggelos Xomalis[2], Maria Farsari[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center Scope, University of Stuttgart, Stuttgart, Germany — [2]Institute of Electronic Structure and Laser - Foundation for Research and Technology Hellas (IESL-FORTH), Heraklion, Greece

Direct Laser Writing (DLW) by two photon absorption has proven to be a versatile technique for the creation of arbitrary solid 3D polymer nanostructures for photonics, biomedical and microfluidic applications. By employing laser intensities that are only slightly above the nonlinear polymerization threshold, structures with submicron resolution can be fabricated.

In this work, we combine DLW and subsequent electroless silver plating to experimentally and theoretically study the plasmonic version of a 3D chiral meta-atom, which comprises of a loop-wire structure or the so-called twisted omega particle. In this case, the metallic wire of finite length supports an electric dipole, whereas the loop acts as a split ring resonator which exhibits a magnetic dipole resonance leading to the separation of right handed circularly polarized light (RCP) and the left-handed one (LCP). FTIR spectroscopy is utilized to electromagnetically characterize the fabricated structures for both circular and linearly polarized waves demonstrating strong CD response in the IR region in accordance with theoretical predictions.

O 60: Chemistry at Solid/Liquid Interfaces

Time: Wednesday 15:00–18:15 Location: S052

Invited Talk O 60.1 Wed 15:00 S052

First-principles photo-electrocatalysis beyond the computational hydrogen electrode — •Harald Oberhofer — Technische Universität München, Germany

First-principles based computational modelling assumes an ever increasing role in understanding and partly already optimising catalysts for photo-electrochemical reactions. The success of prevalent approaches like the computational hydrogen electrode (CHE) thereby relies largely on a numerical efficiency sufficiently high as to allow for large-scale screening of catalyst materials. Such efficiency arises out of well chosen descriptors that ideally condense the mechanistic understanding of the ongoing catalytic reactions at the solid-liquid interface.

In recent years, there is increasing evidence that this understanding needs further scrutiny. Critical aspects in this respect are the neglect of solvation effects, the assumption of pathways that exclusively proceed via proton-coupled electron transfer steps, and the neglect of any kinetic limitations in the CHE approach. In this talk I will review our recent activities in addressing these issues with detailed first-principles based multiscale modeling approaches. Thereby, in particular embedding approaches—both on the solid and the liquid side of the interface—have the potential for a refined description without sacrificing computational efficiency.

O 60.2 Wed 15:30 S052

Continuum embedding for photo-electrochemical surface processes — •Markus Sinstein[1], Harald Oberhofer[1], Daniel Berger[2], Volker Blum[3], and Karsten Reuter[1] — [1]TU München — [2]University of California, Los Angeles — [3]Duke University

The problem of global warming has been known for decades and is believed to be linked directly to the exhaust of carbon dioxide and other gases into the atmosphere which are produced in the combustion of fossil fuel. Carbon-neutral energy sources can be obtained by converting abundant sunlight into chemical compounds. Prominent examples for photo-electrochemically driven reactions generating solar-fuel are the water splitting reaction and the carbon dioxide reduction at metal-oxide solid photo-catalysts. A detailed analysis of the involved elementary processes via first-principles calculations is challenging due to the necessity to simultaneously account for the extended semiconductor surface and the liquid electrolyte. Going beyond traditionally assumed proton-coupled electron transfer mechanisms one may furthermore face charged intermediate states where a significant stabilization due to the polar liquid environment is to be expected. This necessitates a method able to capture electrostatic solvent effects whilst being computationally inexpensive in order to allow for efficient catalyst screening. To this end, we implemented an implicit solvation scheme based on the multipole expansion method into the density functional theory package FHI-aims and discuss first investigations on the photo-electro-catalytic oxygen evolution reaction on rutile titanium dioxide surfaces.

O 60.3 Wed 15:45 S052

Molecular dynamics simulations of the libration region of the SFG spectra at the water-air interface. — •Rémi Khatib[1], Taisuke Hasegawa[2], Marialore Sulpizi[1], Ellen H. G. Backus[3], Mischa Bonn[3], and Yuki Nagata[3] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Department of Chemistry, Graduate School of Science, Kyoto University, Kyoto, Japan — [3]Department for Molecular Spectroscopy, Max Planck Institute for Polymer Research, Mainz, Germany

Sum-frequency generation spectroscopy (SFG) has been used to probe interfacial water structure. Former studies of the stretching and bending modes have evidenced, that non-hydrogen-bonded O-H groups are present at the water-air interface.[1,2] In contrast, the low-frequency librational mode has been much less studied.

In this study, we compute the SFG spectrum at the water-air interface in the libration region by using molecular dynamics simulations. We show that the modelling of the polarizability for the optical response calculation has a drastic effect on the simulated spectra, while force field and dipole models have a minor impact. At the water-air interface, the neighbouring hydrogen-bond partner affects the polarizability in a very heterogeneous way, which cannot be captured with a single point polarizability model per water molecule. In the simulated spectra, the peak of the librational contribution to the imaginary part of the response is centred at 660 - 750 cm^{-1}.

[1] Du, Q. *et al.*, Phys. Rev. Lett., 1993, 70, 2313-2316. [2] Nagata, Y. *et al.*, J. Phys. Chem. Lett., 2013, 4, 1872-1877

O 60.4 Wed 16:00 S052

Towards First-Principles Modeling of Electrolytic Solvent Effects in Photo-Catalytic Water Splitting — •Stefan Ringe[1], Harald Oberhofer[1], Sebastian Matera[2], and Karsten Reuter[1] — [1]Technische Universität München — [2]Freie Universität Berlin

Due to the complexity of the physical processes underlying photocatalytic surface reactions, ab-initio computational approaches have to overcome major challenges concerning accuracy and computational costs. In particular, an efficient description of electrolytic solvent effects - which are crucial for charge driven reactions - is highly necessary. We present an implementation of the modified Poisson-Boltzmann (MPBE) model in the highly parallel and numerically efficient all-electron DFT code FHI-aims.[1] In contrast to most implicit solvent models, this technique combines dielectric solvent response with a mean-field description of solvated finite-sized ions. This has been shown to capture a majority of electrochemical solvent effects appearing in heterogeneous photo-catalysis.[2] We developed a Newton method by linearizing the MPBE and solving the resulting linearized Poisson-Boltzmann Equation (LPBE) by a self-consistent function-space oriented solution scheme which in contrast to common multi-grid solvers is able to exploit the specialized grids and optimized integration schemes of FHI-aims. We demonstrate the approach and its efficiency by investigating hydration and ionic effects on the solvation properties of a wide range of neutral molecules and ions.

[1] Blum, V. et al.,Comp. Phys. Comm. 2009, 2175-2196. [2] e.g. Kilic, M.S., Bazant, M.Z., Phys. Rev. E, 2007, 021502.

O 60.5 Wed 16:15 S052

What quantum dynamics tells us about photocatalytic water splitting — •Jan Mitschker and Thorsten Klüner — Carl-von-Ossietzky-Universität, Oldenburg, Germany

Combining quantum chemistry with quantum dynamics is a valuable tool to simulate processes on a femtosecond time scale. In this contribution, the focus is on the photochemistry of water on a rutile (110) surface. Highly accurate potential energy surfaces for the adsorption of water on rutile were calculated on a CASSCF level of theory. The rutile surface is modelled by a cluster embedded in a large point charge field. The electronically excited state resulting from a hole attack on the water molecule was simulated by a positively charged adsorbate. From about 170000 data points for each state the potential energy surfaces were constructed using artificial neural networks for the interpolation.

Two photoreactions were studied: photodesorption and photodissociation. Numerical wave-packet propagation solves the time-dependent Schrödinger equation and accounts for all quantum effects. Our results indicate an MGR mechanism for the desorption due to the repulsive interaction between adsorbate and substrate in the excited state. Describing the photodissociation, however, is much more complicated due to the underlying Hamiltonian. Using a simpler two-dimensional model, the process is dominated by an energy barrier near the Franck-Condon region leading to a splitting of the wave-packet and introducing strong isotope effects.

O 60.6 Wed 16:30 S052

First-principles reaction barriers for the splitting of water on rutile TiO_2 (110) — •Thomas Stecher, Harald Oberhofer, and Karsten Reuter — TU München, Garching, Deutschland

First-principles modelling of electrocatalytic surface reactions is still largely defined by the computational hydrogen approach. This approach evaluates free energy differences between consecutive reaction steps and thereby accounts only for thermodynamic barriers. In order to access additional kinetic barriers in the photocatalytic oxidation of water we present an approach based on *ab initio* molecular dynamics (AIMD) simulations and umbrella sampling. As a first showcase system we consider the initial proton-transfer step during water-splitting on a rutile TiO_2 (110) surface, which was previously studied within the computational hydrogen electrode approach [1]. AIMD on a system of this size is enabled by an electrostatic embedding approach of both the solid and liquid parts of the reaction site. Furthermore it was found to be imperative that the rearrangement of water, which plays a key role, be considered in the definition of the reaction coordinate. This is achieved by an energy-based reaction coordinate inspired by Marcus theory. Finally, hybrid-level DFT functionals are required for a realistic description particularly of the transition state. Bringing these computational ingredients together allows us to disentangle thermodynamic and kinetic contributions to the reaction barrier. [1] H. Oberhofer and K. Reuter, J. Chem. Phys. **139**, 044710 (2013).

O 60.7 Wed 16:45 S052

Structure Sensitivity of the Oxygen Evolution Reaction on Cobalt(II,III) Oxide — •Craig Plaisance[1], Karsten Reuter[1], and Rutger van Santen[2] — [1]Technische Universität München, Germany — [2]Technische Universiteit Eindhoven, The Netherlands

Quantum chemical calculations and kinetic simulations were used to examine the structure sensitivity of the oxygen evolution reaction on several surface terminations of Co_3O_4 [1]. Three characteristically different active sites were identified, all of which carry out O-O bond formation by nucleophilic attack on an oxo coordinated by one to three Co cations. A method was developed to calculate the turnover frequency of oxygen evolution as a function of overpotential, and it was found that three overpotential ranges exist, each with a different active site dominating. At low overpotentials an oxo coordinated to two Co(IV) and one Co(II) at a step edge of the (311) surface is most active. At medium overpotentials, the active site switches to an oxo coordinated to two Co(IV) on the A termination of the (110) surface, and at high overpotentials, to an oxo coordinated to a single Co(V) on the B termination of the (110) surface. The less coordinated oxos are intrinsically more reactive but require a higher overpotential to oxidize to the active state. Analysis of the electronic structure indicates that the intrinsic reactivity is related to the energy to transfer a hole from an oxidized Co cation to the oxo, with the less coordinated sites requiring the least energy.

[1] C.P. Plaisance and R.A. van Santen, *J. Am. Chem. Soc.*, 2015, *137* (46), 14660-72.

O 60.8 Wed 17:00 S052

Improved Chemical and Electrochemical Stability on Perovskite Oxides by Oxidizing Cations at the Surface — Qiyang Lu[1], Nikolai Tsvetkov[1], Lixin Sun[1], Ethan Crumlin[2], and •Bilge Yildiz[1] — [1]Massachusetts Institute of Technology, Cambridge MA, USA — [2]Lawrence Berkeley National Laboratory, Berkeley CA, USA

Segregation and phase separation of aliovalent dopants on perovskite oxide (ABO3) surfaces is detrimental to the performance of electrocatalytic energy conversion systems such as solid oxide fuel/electrolysis cells and catalysts for thermochemical H2O and CO2 splitting. One key reason behind the instability of perovskite oxide surfaces is the electrostatic attraction of the negatively charged A-site dopants (Sr2+ on La3+ site) by the positively charged oxygen vacancies enriched at the surface. Here we take La0.8Sr0.2CoO3 (LSC) as a model perovskite oxide, and modify its surface with additive cations that are more and less oxidizing than Co on the B-site of LSC. We utilized ambient pressure X-ray absorption and photoelectron spectroscopy to prove that the dominant role of the oxidizing surface additives is to suppress the enrichment and phase separation of Sr while reducing the concentration of oxygen vacancies at the surface. Consequently, we found the effect of these oxidizing cations to be significantly improved stability, with up to 30x acceleration of the oxygen exchange kinetics. Finally, the results revealed a *volcano* relation between the oxygen reduction reaction (ORR) kinetics and the oxygen vacancy formation enthalpy of the binary oxides of the additive cations.

O 60.9 Wed 17:15 S052

Enhancement of electrocatalytical activity for oxygen evolution in bimetallic tetrapyridyl-porphyrine networks — Benjamin Wurster[1], Doris Grumelli[1], •Diana Hötger[1], Rico Gutzler[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne

Hydrogen and oxygen generated by electrochemical water splitting offers a source of clean and renewable energy. The limiting factor is the oxygen evolution reaction (OER) which is a demanding reaction as it involves a four-electron transfer ($4\,OH^- \rightarrow O_2 + 2\,H_2O + 4\,e^-$, in alkaline electrolytes). As a result, the reaction has to overcome a large overpotential. Inspired by the reactivity of single metal atom catalysts and the structure of metallo-proteins, a bimetallic porphyrine catalyst for the OER was fabricated. Tetrapyridyl prophyrines provide two different coordination environments for the stabilization of single metal centers: the porphyrine ring and the pyridyl groups. Using this method we intentionally place Co and Fe atoms in either of the two coordination environment within a porphyrine monolayer on Au(111).

Compared to the single metal porphyrines the bimetallic networks show an increase in activity towards oxygen production of approximately two orders of magnitude. The enhancement of the activity is due to a cooperative effect between the metal centers positioned in the two coordination environments. Additionally, the reaction starts with an overpotential of about 300 mV, highlighting the favorable kinetics of the catalyst.

O 60.10 Wed 17:30 S052

Electro-oxidation of methanol from first-principles with an implicit solvation method — •Sung Sakong and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The methanol electro-oxidation is the central reaction in the direct methanol fuel cell (DMFC). We present a first-principles computational studies addressing the reaction mechanism occuring on the anode of the DMFC based on density functional theory (DFT). The electrode-electrolyte interface is modeled by a Pt(111) slab in an implicit solvent [J. Chem. Phys. **142**, 234107 (2015)]. The electrode potential of the electrochemical cell is parametrized using the computational hydrogen electrode method. Thus DFT calculations yield the energetics of reaction intermediates on the Pt electrode as a function of the electrode potential U. We find that the presence of the implicit solvent leads to subtle changes in the relative energies of the reaction intermediates. Based on calculated activation barriers, a possible reaction scheme is proposed. We will demonstrate that the total oxidation of methanol is possible at electrode potentials of $U > 0.6\,\mathrm{V}$ on Pt(111), in agreement with experimental observations. Based on the proposed reaction scheme, we will discuss possible scenarios to improve the performance in the methanol electro-oxidation.

O 60.11 Wed 17:45 S052

Electro-oxidation of methanol and CO on UHV prepared Pt modified Ru(0001) model electrodes — •Jens Klein, Fabian Argast, Albert K. Engstfeld, Sylvain Brimaud, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany

Bimetallic platinum-ruthenium catalysts are the state-of-the-art anode electrode materials for direct methanol fuel cells, since they show a much higher activity towards both the methanol (MeOH) oxidation and the CO oxidation compared to the standard anode catalyst Pt. The higher activity has been ascribed to adjacent bimetallic PtRu-sites (‚bifunctional mechanism‘). The actual structure of the active sites remained, however, unclear.

For a more detailed understanding of the structure–activity relationship of this system, we investigated these reactions on structurally well-defined nanostructured bimetallic Pt modified Ru(0001) surfaces in a combined ultrahigh vacuum (UHV) – electrochemical (EC) flow cell setup. Different Pt- and PtRu-nanostructures with varying Pt coverage and varying number of adjacent PtRu-sites were prepared by physical vapor deposition of Pt on Ru(0001) at different temperatures and then characterized by scanning tunneling microscopy (STM).

After structural analysis, the model electrodes were transferred to an EC flow cell attached to the UHV system, to investigate their electrocatalytic activity during MeOH oxidation and bulk CO oxidation in H_2SO_4 by cyclic voltammetry. The electrocatalytic activity was correlated with the abundance of key PtRu nanostructures on the surfaces.

O 60.12 Wed 18:00 S052

Equilibrium coverages of ions on metals electrodes — •Florian Gossenberger, Tanglaw Roman, and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

Electrocatalytic reactions typically take place close to the surface of the electrode, i.e., in the region of the electrochemical double layer. These reactions might be substantially affect by adsorbates on the electrode which originate from the electrolyte. They can contribute to catalytic steps by directly interacting with the reactants, by changing the work function, or simply by blocking adsorption sites on the surface.

In this study we have addressed the equilibrium coverage of ions on Pt(111) in the presence of electrolytes using density functional theory. By applying the concept of the computational hydrogen electrode, we have derived the stability of structures at the electrode surface at different electrochemical potentials which are a function of electrode potential, pH, ion concentrations and temperature [1].

With this information we are able to draw phase diagrams for several coadsorption systems. Thereby we can address the open question whether synergistic effects are present in coadsorption systems of halides (Cl^-, Br^-, I^-) and hydrogen on Pt(111). Our results indicate that the adsorption of these species is competetive, i.e., that either purely hydrogen-covered or purely halide-covered phases are stable.

[1] F. Gossenberger, T. Roman, A. Groß, Surf. Sci. **631**, 17 (2015).

O 61: Graphene II: Adsorption, Intercalation and Doping

Time: Wednesday 15:00–18:00 Location: S053

O 61.1 Wed 15:00 S053

H atom scattering from epitaxial graphene on Pt(111) — •Hongyan Jiang[1], Yvonne Dorenkamp[1], Alec Wodtke[1,2,3], and Oliver Buenermann[1,2,3] — [1]Institute for Physical Chemistry, Georg-August University of Goettingen, Goettingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, Goettingen, Germany — [3]International Center for Advanced Studies of Energy Conversion, Georg-August University of Goettingen, Goettingen, Germany

Adsorption of hydrogen atoms on graphene is playing an important role in hydrogen storage, graphene based electronics, nuclear fusion and interstellar chemistry. The interaction of hydrogen atoms with graphene is studied in a newly built atom-surface scattering machine. A nearly mono-energetic hydrogen atom beam is formed by laser photolysis. The hydrogen atoms are scattered from a well-defined sample held in UHV. The scattered hydrogen atoms are detected using Rydberg-atom neutral time-of-flight. This technique allows us to record angle resolved, high resolution energy loss spectra of scatted hydrogen atoms. Scattering of hydrogen atoms from epitaxial graphene on Pt(111) shows a very different behavior than scattering from clean Pt(111). For low incidence kinetic energy, graphene acts like an atomic mirror. We observe narrow scattering angle and kinetic energy distribution and small translational energy loss. For high incidence kinetic energy, broad distribution and large translational energy loss is observed. The process obeys normal energy scaling. We speculate that this behavior is connected to the barrier of hydrogen atom adsorption on graphene.

O 61.2 Wed 15:15 S053

A nanodiamond superlattice on graphene/Ir(111) — •Charlotte Herbig[1], Philipp Valerius[1], Timo Knispel[1], Sabina Simon[1,2], Ulrike A. Schröder[1], Antonio J. Martínez-Galera[1], Mohammad A. Arman[3], Christian Teichert[1,4], Jan Knudsen[3,5], Arkady V. Krasheninnikov[6,7], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Department of Physics, University of Konstanz, Germany — [3]Division of Synchrotron Radiation Research, Lund University, Sweden — [4]Institute of Physics, Montanuniversität Leoben, Austria — [5]MAX IV Laboratory, Lund, Sweden — [6]Department of Applied Physics, Aalto University, Finland — [7]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany

Atomic C deposition onto the graphene moiré with Ir(111) leads in a broad temperature range from 130 K to 550 K to the formation of a nanodiamond superlattice with one C cluster per moiré unit cell. The size of the C clusters is tunable between about 20 and 150 C atoms. For deposited amounts exceeding about 200 C atoms per moiré unit cell the ordering is lost, but still nanodiamond structures remain. The nanodiamond superlattice is thermally stable up to 800 K. Annealing to higher temperatures results in C intercalation and eventually bilayer graphene formation. On the basis of scanning tunneling microscopy, X-ray photoelectron spectroscopy, and density functional theory a model for C cluster formation, structure, stability, and decay is developed. Based on the generality of our model, we speculate that nanodiamonds may form on other moirés of 2D materials with their substrate.

O 61.3 Wed 15:30 S053

Core level shifts of doped graphene — •Ulrike A. Schröder[1], Marin Petrović[2], Timm Gerber[1], Elin Grånäs[3], Antonio J. Martínez-Galera[1], Mohammad A. Arman[3], Charlotte Herbig[1], Joachim Schnadt[3], Marko Kralj[2], Jan Knudsen[3,4], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut za fiziku, Zagreb, Croatia — [3]Division of Synchrotron Radiation Research, Lund University, Sweden — [4]MAX IV Laboratory, Lund, Sweden

In X-ray photoemission spectroscopy, core level shifts of the carbon 1s photoelectrons are frequently monitored to investigate adsorption and intercalation on and underneath graphene. An understanding of their origin and magnitude are thus desirable both from a scientific and an applicational point of view. Through intercalation of metals and gases, the Dirac cone of graphene on Ir(111) can be shifted with respect to the Fermi level without becoming destroyed through strong hybridization. Upon such chemical doping with Cs, Eu, H, O, and Li, the carbon 1s core level shift displays a functional dependence on the graphene doping level. Of specific interest is the case of doping by Li, since for Li no phase separation takes place upon intercalation. Thereby, this core level shift can be monitored as a function of the intercalated amount. To first approximation, the core level shift may be described as a superposition of a rigid band shift, which is counteracted by a shift proportional to the transferred charge.

O 61.4 Wed 15:45 S053

Structural phases of Au-intercalated graphene on Ni(111) — •Maxim Krivenkov[1,2], Evangelos Golias[1], Dmitry Marchenko[1], Jaime Sánchez-Barriga[1], Gustav Bihlmayer[3], Oliver Rader[1], and Andrei Varykhalov[1] — [1]Helmholtz-Zentrum Berlin, BESSY-II, 12489, Berlin, Germany — [2]Department of Physics, Potsdam University, Am Neuen Palais 10, D-14415, Potsdam, Germany — [3]Forschungszentrum Jülich and JARA, 52425, Jülich, Germany

Graphene grown epitaxially on Ni(111) and intercalated with Au is a remarkable system revealing a giant (∼100 meV) spin-orbit splitting of Dirac cone in spin-resolved photoemission experiments [1]. In present study we investigate structural origin of this giant Rashba effect. We report extensive microscopic study of Au-intercalated graphene and discover versatile structural phases of Au locally coexisting at graphene-Ni interface. Besides a continuous monolayer phase giving rise to a pronounced moiré pattern identified as (9.7×9.7) misfit dislocation loop structure [2], we observe various well periodic arrays of nanoparticles trapped under graphene. Overall arrangement of such Au nanoclusters is laterally coherent to the principle moiré pattern of Au monolayer. We test whether these nanoparticles can be a source of giant spin-orbit splitting in graphene by performing DFT study of structural and electronic properties of the system.

[1] D. Marchenko, A. Varykhalov, M. R. Scholz, G. Bihlmayer, E. I. Rashba, A. Rybkin, A. M. Shikin, O. Rader, Nature Commun. 3, 1232 (2012); [2] J. Jakobsen et al., Phys. Rev. Lett. 75, 489 (1995).

O 61.5 Wed 16:00 S053

How to manipulate the dispersion interaction at organic-graphene interfaces — •Vasile Caciuc[1], Felix Huttmann[2], Nicolae Atodiresei[1], Thomas Michely[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

In this contribution we will explore how to rationally engineer the strength of the van der Waals (vdW) interactions present in a molecule–surface physisorbed system. More specifically, we investigated by means of *ab initio* density functional theory (DFT) simulations using a non-local correlation vdW functional [1] the adsorption of a $\pi-$conjugated organic molecule such as naphthalene ($C_{10}H_8$) on the graphene/Ir(111) surface [2]. To tailor the magnitude of the naphthalene–graphene dispersion interaction, the key ingredient is to modify the spatial extent of the charge distribution in graphene by doping it via intercalated electropositive and electronegative atoms at its backside to Ir(111) [3]. Finally, the comparison of the predicted adsorption energies and those obtained by thermal desorption measurements is also discussed [4].

[1] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).
[2] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).
[3] S. Schumacher *et al.*, Nano Lett. **13**, 5013 (2013).
[4] F. Huttmann *et al.*, Phys. Rev. Lett., accepted.

O 61.6 Wed 16:15 S053

Coverage dependent evolution of electronic states of tetraphenyldibenzoperiflanthene (DBP) on HOPG and graphite — •Tobias Huempfner[1], Tino Kirchhuebel[1], Roman Forker[1], Noriaki Kawakita[2], Takashi Yamada[2], Toshiaki Munakata[2], and Torsten Fritz[1,2] — [1]Friedrich Schiller University, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Department of Chemistry, Graduate School of Science, Osaka University, 1-1 Machikaneyama, Toyonaka 560-0043, Osaka, Japan

We report on a combined study of the dye molecule tetraphenyldibenzoperiflanthene (DBP) deposited on HOPG and single crystalline graphite surfaces. The film growth is successively traced in situ via differential reflectance spectroscopy (DRS). This data is compared to ultraviolet photoelectron spectroscopy (UPS) as well as two photon photoemission (2PPE) measurements recorded at various coverages. All methods applied show that there are two different species of the DBP molecule that appear at certain film thicknesses. For low coverages, namely up to one monolayer (ML), the absorption gap of the molecules is smaller (low energy - LE) compared to coverages slightly above 1 ML (high energy - HE). For thicker films up to 10 ML the LE species is formed again and the film composition shifts continuously in favor of this species with increasing coverage. This study is assisted by structural data gained from low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) that depicts a highly ordered first ML.

O 61.7 Wed 16:30 S053

Supramolecular nanopatterns of organic molecules on graphite — •Stefan-Sven Jester — Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn

The self-assembly of organic molecules at the solid/liquid interface provides an approach towards defined 2D architectures. However, predicting how a specific molecule renders into a supramolecular 2D crystal is still a challenge. A promising approach relies on the transfer of concepts from discrete geometry (e.g. Archimedean surface tiling) to supramolecular chemistry: Arylene-alkynylene macrocycles of distinct symmetries and sizes that carry flexible alkyl/alkoxy side chains can be viewed as molecular polygons that form supramolecular patterns of specific symmetries and lattice constants. E.g., the cocrystal of molecular triangles and hexagons has increased lattice constants as compared to the individual compounds. We describe a concentration-driven alteration between porous and dense packings of hexagons with reduced symmetry and alike unit cell parameters for rings with different interiors. In addition, we discuss mono- and multilayer growth of molecular spoked wheels on graphite. In all cases, scanning tunneling microscopy provides a submolecularly resolved insight into the molecular structures that can be utilized for chemical compound analysis.

O 61.8 Wed 16:45 S053

Molecular friction and proton dynamics in sulfuric acid intercalated graphite from ab-initio MD simulations — •Steffen Seiler and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Wet-chemical exfoliation of graphite via Hummers' method [1,2] is a promising route for large-scale graphene production. In this solution-based process first graphite is intercalated by concentrated sulfuric acid, then the graphite intercalation compound (GIC) is oxidized, graphene oxide (GO) layers are separated in solution by hydrolysis reactions, and finally the GO layers are reduced to graphene [3].

We performed Car-Parrinello molecular dynamics (CP-MD) simulations to study the dynamic properties of the liquid sulfuric acid within the confined space between the graphene layers. The friction coefficient, proton-transfer barriers and electron distributions have been analyzed, and we will show how these properties are affected by the oxidation and the stacking sequence of the graphene sheets. Finally, consequences for the mechanism of GIC formation and oxidation will be discussed.

[1] W. S. Hummers, *J. Am. Chem. Soc.* **80**, 1339 (1958).
[2] D. C. Marcano et al., *ACS Nano* **4**, 4806 (2010).
[3] A. M. Dimiev and J. M. Tour, *ACS Nano* **8**, 3060 (2014).

O 61.9 Wed 17:00 S053

Surface mediated oxidation of supported coronene molecules — •Weippert Jürgen[1], Gewiese Vincent[1], Böttcher Artur[1], and Kappes Manfred M.[1,2] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

We have explored surface-mediated oxidation of coronene (C24H12) molecules as a route to prepare molecular equivalents of graphene oxides (GOs). We found that exposure of C24H12/HOPG to a flux of atomic oxygen leads to oxidation of both the substrate and the coronene molecules adsorbed thereon (O/HOPG and C24H12On). We did not observe molecular fragments indicative of epoxy-species induced unzipping and scission of the adsorbed coronene. Instead desorption mass spectra were dominated by Coronene molecules deriving from electron impact ionization of the intact parent species, two oxidic species and an unusual coronene fragment, C21H9+. These observations suggest that sample heating activates the surface diffusion of preformed epoxy species and that subsequently pronounced fragmentation of the oxidized molecular periphery is induced either by further on-surface heating or by ionization. The reaction path results in the emission of coronene oxides with a mean yield of 0.07. Systematic measurements (TDS, UPS and XPS) reveal further details of the reaction chain associated with efficient thermal desorption of coronene oxides - a process analogous to the exfoliation of graphene oxide.

O 61.10 Wed 17:15 S053

Intercalation of Gadolinium underneath graphene on SiC(0001) — •Stefan Link, Stiven Forti, Alexander Stöhr, and Ulrich Starke — Max-Planck-Institut für Festkörperforschung Stuttgart

Tuning the electronic properties of graphene for potential applications has raised intensive research. Besides spatial confinement for the introduction of a band gap or covalent functionalization, the intercalation of foreign atom species is a promising approach. A highly interesting state of graphene lies in the extreme doping regime, where a van-Hove singularity is reached at the Fermi level. Although this is a rather difficult task, it might pave the way to introduce interesting effects like superconductivity. Gating is illusional for this purpose due to the lack of appropriate dielectrica. Notably, the introduction of dopant adatoms like alkali and/or earth alkali metals onto both sides of the graphene leads to success but on the cost of strongly reduced stability. Here we show in a different approach that such a system can be produced with strong thermal and chemical stability. The system develops by intercalating Gadolinium atoms beneath the so called zerolayer graphene on SiC(0001). We make use of the advanced fabrication of epitaxial graphene on SiC(0001) in our group to achieve homogeneous results on a large scale. This gives the opportunity for exploring graphene's properties in this exotic regime. We show that reaching this regime is accompanied by strong renormalization effects in the electronic band structure, which are partially driven by strong electron-phonon coupling.

O 61.11 Wed 17:30 S053

Transformation of metallic boron into substitutional dopants in graphene on 6H-SiC(0001) — •Jessica Sforzini[1,2], Mykola Telychko[3,4], Ondrej Krejcio[3,4], Martin Vondracek[5], Martin Svec[3], Francois Bocquet[1,2], and Stephan Tautz[1,2] — [1]Peter Gruenberg Institut (PGI-3), Forschungszentrum Juelich, 52425 Juelich, Germany — [2]Juelich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Juelich, Germany — [3]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, CZ-16200 Prague, Czech Republic — [4]Faculty of Mathematics and Physics, Charles University, V Holesovickach 2, Praha 8, Czech Republic — [5]Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 10, CZ-18228 Prague, Czech Republic

We investigate the development of the local bonding and chemical state of boron atoms during the growth of B-doped graphene on 6H-SiC(0001). Photoemission experiments reveal the presence of two chemical states, namely boron in the uppermost SiC bilayers and boron substituted in both the graphene and buffer layer lattices. We demonstrate the participation of the dopant in the π^* electron system of graphene by the presence of the π^* resonance in the near edge x-ray adsorption fine structure (NEXAFS) recorded at the B K-edge. The experimental fundings are supported by NEXAFS simulations.

O 61.12 Wed 17:45 S053

Chemical modification of bilayer graphene — •Konstantin Weber and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Using density functional theory (DFT) together with the empirical Grimme D2 van der Waals correction scheme [1] we studied the energetics, reaction pathway and thermodynamics of the hydroxylation and hydrogenation reaction and subsequent interlayer bond formation in bilayer graphene. Our results show that after the adsorption of two to three adsorbates a critical nucleous size is reached and subsequent adsorption leads to an energy gain for both the adsorption of hydrogen and hydroxyl groups. The covalent adsorption increases the reactivity of bilayer graphene and triggers the formation of interlayer bonds between the graphene sheets. In addition, the reactivity of freestanding bilayer graphene will be compared to the reactivity of bilayer graphene adsorbed on a Ni(111) substrate. The Ni(111) surface acts as a support and reaction template that facilitates the hydrogenation and hydroxylation reactions, similarly as in the one-sided hydrogenation process of single-layer graphene supported on Ni(111) [2].

[1] S. Grimme, *J. Comp. Chem.* **27**, 1787 (2006).
[2] W. Zhao et al., *Chem. Eur. J.* **21**, 3347 (2015).

O 62: Frontiers of Electronic Structure Theory: Focus on Topology and Transport III

Time: Wednesday 15:00–18:30 Location: H24

Topical Talk O 62.1 Wed 15:00 H24

Topological semimetal phases in strained HgTe-based alloys — Tomáš Rauch[1], Steven Achilles[1], •Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Topological insulators (TIs) have matured to a class of materials that is studied worldwide with great effort. Prominent examples are HgTe, the Bi chalcogenides, and SnTe. Recently, the set of "original" TIs has been extended by topological semimetals: the topological Dirac and the Weyl semimetals, both of them showing point-like Fermi surfaces in the bulk. Weyl points appear always in pairs with opposite topological charges of ±1; their projections onto the surface Brillouin zone are connected by a Fermi arc, i. e. a sizably spin-polarized topological surface state with an open Fermi contour.

In this presentation I report on theoretical investigations of strained $\mathrm{HgTe}_{1-x}\mathrm{S}_x$ alloys [1], with surprising results. (*ı*) In the strong TI phase, the spin chirality of the topological nontrivial surface state can be reversed by moderate strain and changing the alloy concentration x. (*ıı*) On top of this, we observe a Dirac and a Weyl semimetal phase. These findings call for experimental verification and extend significantly the "topological playground" for spin-dependent transport.

[1] T. Rauch, S. Achilles, JH, I. Mertig, Phys. Rev. Letters **114** (2015) 236805.

Topical Talk O 62.2 Wed 15:30 H24

Topological surface Fermi arcs and the chiral anomaly in Weyl semimetal materials — •Binghai Yan — Max Planck Institute for Chemical Physics of Solids, Dresden

Topological Weyl semimetals represent a novel state of topological quantum matter, which not only possesses Weyl fermions (massless chiral particles that can be viewed as magnetic monopoles in momentum space) in the bulk and unique Fermi arcs generated by topological surface states, but also exhibits appealing physical properties such as extremely large magnetoresistance and ultra-high carrier mobility. In this talk, I will first present our recent theoretical [1] and ARPES [2,3] study on the topological surface states of transition-metal monopnictides, NbP, NbAs, TaP and TaAs. By visualizing the surface Fermi arcs, we discovered their Fermiology evolution with spin*orbit coupling strength. Further, we found a way to manipulate the Fermi arcs by the Lifshitz transition. I will also introduce our recent progress on the magneto-transport in the search for the chiral anomaly effect[4,5]. References: [1] Y. Sun, S. C. Wu, and B. Yan, Phys. Rev. B 92, 115428 (2015). [2] L. X. Yang, et al. Nature Physics 11, 728 (2015). [3] Z. K. Liu, et al. Nature Materials DOI: 10.1038/NMAT4457 (2015). [4] C. Shekhar, et al. Nature Physics 11, 645 (2015). [5] C. Shekhar, et al. arXiv:1506.06577 (2015).

O 62.3 Wed 16:00 H24

Type-II Dirac cones as unified topological origin of the exotic electronic properties of $\mathbf{WTe_2}$ — •Lukas Muechler[1], Aris Alexandradinata[2], Titus Neupert[3], and Roberto Car[1] — [1]Dept. of Chemistry, Princeton University — [2]Dept. of Physics, Yale University — [3]Princeton Center for Theoretical Science, Princeton University

$\mathrm{WTe_2}$ is a recently discovered layered material with remarkable electronic properties. Transport measurements show an extremely large non-saturating magnetoresistance (MR) with mobilities as high as 167 000 $\mathrm{cm^2/Vs}$ at 2 K. Furthermore, recent photoemission experiments discovered circular dichroism in the bulk band structure. We propose a unified explanation for these exotic observations by relating key properties of the bulk electronic structure to that of to that of the mono- and bi-layer material. In particular, we demonstrate that the monolayer is a novel type-II Dirac semimetal in absence of spin-orbit coupling, with Dirac cones that are sufficiently anisotropic to simultaneously harbor electron and hole pockets. The band structure can be characterized by a new $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological invariant defined through non-Abelian Wilson loops. We develop a tight-binding model for the mono- and bilayer of $\mathrm{WTe_2}$ based on Wannier functions from *ab-inito* calculations and extend our findings to the iso-structural compounds $\mathrm{MoTe_2}$ and $\mathrm{ZrI_2}$.

O 62.4 Wed 16:15 H24

Topological surface Fermi arcs and spin-textures of the Weyl semimetals TaAs, TaP, NbAs, and NbP — •Yan Sun[1], Shu-Chun Wu[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Very recently the topological Weyl semimetal (WSM) was predicted in the noncentrosymmetric compounds NbP, NbAs, TaP, and TaAs and soon led to photoemission experiments to verify the presumed topological Fermi arcs (FAs)[1,2]. In this work we have performed fully ab initio calculations of these four WSMs and revealed the FAs with spin-momentum-locked spin texture[3]. On the (001) surface, the anion (P or As) terminated surfaces are found to fit photoemission measurements well. By tracing the spin polarization of the Fermi surface, one can distinguish FAs from trivial Fermi circles. By comparing their surface states, we reveal the evolution of topological Fermi arcs from the spin-degenerate Fermi circle to spin-split arcs when the SOC increases from zero to a finite value. Our work presents a comprehensive understanding of the topological surface states of WSMs, which will be helpful for spin-revolved photoemission and transport experiments.

References

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[3] Y. Sun, S. Wu, and B. Yan, Phy. Rev. B, 92, 115428, (2015).

O 62.5 Wed 16:30 H24

New electron states at the Bi/InAs(111) interface — •L Nicolaï[1,2,3], K Hricovini[2,3], J-M Mariot[4], M C Richter[2,3], O Heckmann[2,3], U Djukic[2], T Balasubramanian[5], M Leandersson[5], J Sadowski[5], J Denlinger[6], I Vobornik[7], J Braun[7], H Ebert[7], and J Minár[7,8] — [1]LMU, Munich — [2]LPMS, UCP, Cergy, France — [3]DSM-IRAMIS, Spec, Cea-Saclay, France — [4]LCP-MR, UPMC Univ. Paris 06/CNRS, France — [5]MAX-lab, Lund Univ., Sweden — [6]ALS, Berkeley, USA — [7]EST, Trieste, Italy — [8]Univ. of West Bohemia, Plzeň, Czech Republic

The Bi(111) surface is a prototype system that shows Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behavior was suggested for a variable film thickness as a function of the layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are quite complex and far from being fully understood. Here we present combined theoretical and ARPES studies on the electronic structure of Bi(111) films grown on InAs(111). Bi grows epitaxially on this substrate and a monocrystal of very high quality is obtained after depositing several monolayers. ARPES experiments on the samples prepared show several new electronic states not reported before. The one-step model of photoemission as implemented in the SPR-KKR package [3] allows us to identify pristine Bi bulk states coexisting with InBi surface states.[1] M. Wada et al., Phys. Rev. B 83, 121310 (2011). [2] Z. Liu et al., Phys. Rev. Lett. 107, 136805 (2011). [3] J. Braun, Rep. Prog. Phys. 59, 1267-1338 (1996).

O 62.6 Wed 16:45 H24

Two-dimensional topological phases and electronic spectra of topological insulator thin films from *GW* calculations — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

We have investigated topological and electronic properties of thin films of the topological insulators Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 with thicknesses from one to six quintuple layers employing the *GW* method. The quasiparticle band structures show highly improved agreement with experiments compared to DFT. In addition to a correction of the band gaps, the energetic positions and dispersions of the surface states change significantly around $\bar{\Gamma}$ [1]. The common approach of taking the diagonal elements of the self-energy Σ as quasiparticle energies and leaving the wave functions unchanged yields unphysical results which can be overcome by diagonalizing $\mathcal{H}^{\mathrm{QP}}$. The origin of the respective off-diagonal elements in $(\Sigma - V_{xc})$ will be discussed. As the wave functions are updated, the two-dimensional topological phases (quantum spin Hall or trivial) in *GW* differ from DFT for many systems. On the basis of our results, we further argue that one cannot unambiguously conclude the topological phase from fits to ARPES band structures as performed in recent experimental studies.

[1] T. Förster, P. Krüger, and M. Rohlfing, Phys. Rev. B **92**, 201404(R) (2015)

O 62.7 Wed 17:00 H24

Steady-State Density Functional Theory for Finite Bias Conductances — •Stefan Kurth[1,2] and Gianluca Stefanucci[3,4] — [1]Dept. of Materials Physics, Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]Dept. of Physics, Univ. of Rome "Tor Vergata", Rome, Italy — [4]INFN, Frascati, Italy

In the framework of density functional theory a formalism to describe electronic transport in the steady state is proposed which uses the density on the junction and the steady current as basic variables. In a finite window around zero bias, a one-to-one map is established between the basic variables and both local potential on as well as bias across the junction. The resulting Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias. For weakly coupled junctions the xc potentials exhibit steps in the density-current plane which are shown to be crucial to describe the Coulomb blockade diamonds. At small currents these steps emerge as the equilibrium xc discontinuity bifurcates. The formalism is applied to a model benzene junction, finding perfect agreement with the orthodox theory of Coulomb blockade.

O 62.8 Wed 17:15 H24

Revealing the intra-molecular origin of inelastic electron tunneling signal by means of first-principles calculations — •Giuseppe Foti and Hector Vazquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Prague, Czech Republic

We explore the intra-molecular contributions to the peaks in the Inelastic Electron Tunneling Spectrum (IETS) of a benzene-based molecular junction by means of DFT-NEGF simulations [1,2]. These contributions are calculated from the bracket of the left- and right- transmission channels with the e-ph coupling matrix by grouping the products into one- and two-atom terms. This combines the geometrical information of the vibrational modes with the electronic properties of the scattering states. Our calculations show how the partial contributions of each atom and bond in the molecule combine to give the total inelastic signal. We find that, for most of the high intensity peaks, these terms sum up constructively while dark modes result from cancellations. We also investigate the relation between the symmetry of the vibrational modes and the cancellation pattern of the different contributions. This analysis enables a real space representation of the intra-molecular contributions associated to each vibrational mode and allows a complete mapping and characterization of the origin of the IETS peaks.

[1] J. M. Soler et al. J. Phys.: Condens. Matter 14, 2745 (2002)

[2] T. Frederiksen et al. Phys. Rev. B 75, 205413 (2007)

O 62.9 Wed 17:30 H24

An efficient real-time time-dependent density functional theory method and its applications — •Zhi Wang[1], Shu-Shen Li[2], and Lin-Wang Wang[3] — [1]Institut für Physikalische Chemie, Uni-Hamburg, Hamburg, Germany — [2]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China — [3]Lawrence Berkeley National Laboratory, Berkeley, United States

We have developed an efficient real-time time-dependent density functional theory (TDDFT) method that can increase the effective time step from <1 as in traditional methods to ~0.1 fs. With this algorithm, the TDDFT simulation can have comparable speed to the Born-Oppenheimer (BO) ab initio molecular dynamics (MD). The application of the method will be illustrated for several non-equilibrium systems, e.g., energetic particle colliding onto a TMDC monolayer, and ultrafast charge seperations in photovoltaic systems.

O 62.10 Wed 17:45 H24

Nonadiabatic geometric phase of a pseudorotating triatomic molecule — •Ryan Requist and Eberhard K. U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The geometric phase of a real-valued Born-Oppenheimer electronic wavefunction is a topological quantity depending on the winding number of the path around a conical intersection of the adiabatic potential energy surfaces in nuclear coordinate space. We report the calculation of a nonadiabatic molecular geometric phase that takes the full quantum mechanical motion of the nuclei into account through the exact factorization scheme [1]. Nonadiabatic contributions "smear out" the point-like adiabatic Berry curvature, changing the topological invariant into a genuine path-dependent geometric phase [2].

[1] S. K. Min, A. Abedi, K. S. Kim and E. K. U. Gross, Phys. Rev. Lett. 113, 263004 (2014). [2] R. Requist and E. K. U. Gross, arxiv:1506.09193.

O 62.11 Wed 18:00 H24

Theoretical investigations of magnetically doped topological insulators — •Jan Minar[1,2], Jurgen Braun[1], and Hubert

Ebert[1] — [1]LMU München, Germany — [2]University of West Bohemia, Plzen, Czech Rep.

Band gap opening of topological surface states due to magnetic doping are the subject of a long standing discussion. However, in spite of the progress made during the last years in this field there are still phenomena that are poorly understood and many open issues to be addressed. In several cases, like for example Mn doped Bi_2Se_3 band gap opening does not seem to be of magnetic origin. Here we will present several examples detailed theoretical studies on various bulk as well as surface doped topological insulators by means of the SPR-KKR band structure method. Our results will be discussed in a direct comparison with the corresponding ARPES [1] as well as XAS and XMCD [2,3] experimental data.

[1] J. Sanchez-Barriga et al., Nat. Communications, submitted (2015) [2] A. Ney et al., in preparation [3] J. Honolka et al., in preparation

O 62.12 Wed 18:15 H24

Trions in a carbon nanotube from ab-initio many-body perturbation theory — •Thorsten Deilmann, Matthias Drüppel, and Michael Rohlfing — Institut für Festkörpertheorie, Universität Münster, Germany

Trion states of three correlated particles (e.g. two electrons and one hole) show up in the optical spectra of doped or gated nanostructures, like carbon nanotubes or transition-metal dichalcogenides.

We demonstrate that trions can be described within ab-initio many-body perturbation theory, as a natural extension of the widely used *GW* method and Bethe-Salpeter equation. This allows for a direct comparison with excitons on equal footing.

We investigate trion states in a semiconducting $(8,0)$ carbon nanotube, and discuss their spectra, composition, and wave functions. Luminescence from the trions is red-shifted by $\sim 135\,\text{meV}$ compared to the excitons.

O 63: Scanning Probe Microscopy and Spin Phenomena

Time: Wednesday 15:00–17:00 Location: H4

Invited Talk O 63.1 Wed 15:00 H4

Spin-orbit coupling, magnetic perturbations, and competing trends in topological insulators — •Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Topological insulators (TIs) interacting with magnetic perturbations lead to several unconventional effects, usually described within the framework of gapping the Dirac quasiparticles due to broken time-reversal symmetry [1,2]. While the quantum anomalous Hall effect confirmes the presence of ferromagnetically gapped Dirac states, the overwhelming majority of photoemission and tunneling data demonstrate the presence of a finite density of states at the Dirac point even once the system becomes magnetic. We present a series of experiments which, by mapping the response of TIs to different magnetic impurities down to the atomic level, provide a detailed microscopic picture and thereby solve these contradictory observations in both surface- and bulk-doped samples. We provide evidence of highly anisotropic Dirac fermion-meditated magnetic interactions that lead to quantum coherent states propagating over mesoscopic distances. We also show that magnetic order and gapless states can coexist due to the emergence of a two-fluid behavior where the competition in between opposite trends, i.e. gap-opening vs. gap-closing, is ultimately linked to the localized vs. delocalized nature of the perturbations-induced quasiparticles.

[1] P. Sessi et al., Phys. Rev. B 88, 161407 (2013).

[2] P. Sessi et al., Nature Comm. 5, 5349 (2014).

Invited Talk O 63.2 Wed 15:30 H4

Conductance and shot noise spectroscopy of single magnetic atoms and molecules — •Alexander Weismann — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel

The scanning tunneling microscope allows to build and study nanostructures at a single atom level. It can be further used to explore the ballistic electron transport regime by bringing the tip into contact with single atoms and molecules in a well-defined way. The measurement of quantum shot noise in nanoscopic contacts provides additional information on the underlying conduction processes and reveals a spin polarization of the current by single Fe and Co atoms between two gold electrodes. The impact of spin-orbit coupling on electron transport is demonstrated using single Ir atoms on a ferromagnetic substrate, where large changes of the anisotropic magnetoresistance occur between the tunneling and the contact regime. On retinoic acid, a closed-shell organic bio-molecules comprising only C, H and O atoms, the STM can be used to reversibly switch the spin state, which is attributed to the conversion into a radical cation.

Invited Talk O 63.3 Wed 16:00 H4

Manipulating spins in single molecules on a superconductor — •Benjamin W. Heinrich — Freie Universität Berlin, Fachbereich Physik, Berlin

The dominant relaxation mechanism for excited spin states on a metal is the exchange of energy and angular momentum with conduction electrons, which results in the creation of electron-hole pairs. A common strategy to increase the spin lifetime consists in reducing the exchange scattering by the introduction of a thin insulating layer between adsorbate and substrate. We propose an alternative route to stabilize excited spin states, which is based on combining a metal-organic complex with a type I superconductor. The organic ligand decreases the exchange scattering with the superconducting quasiparticles sufficiently to avoid screening. In turn, the superconducting gap prohibits the energy transfer to electron-hole pairs when the excitation energy is smaller than the gap. This increases the excitation lifetime for Fe-octaethylporphyrin-chloride to 10 ns when adsorbed on a superconducting lead substrate, which is orders of magnitude longer than when adsorbed on a metal.

Our strategy will enable even longer lifetimes, perhaps sufficiently long to enable coherent spin manipulation, for systems with a well-chosen anisotropy barrier. It turns out that metal-organic complexes might be suited to achieve this goal. They provide structural flexibility such that the ligand field can be reversibly modified by local potentials, *e.g.*, the tip of the STM, which then modifies the magnetic anisotropy. Fine-tuning of the anisotropy appears to be within reach.

O 63.4 Wed 16:30 H4

Voltage-dependent rotational motion of Phthalocyanine molecules — •Andreas Krönlein, Jens Kügel, Paolo Sessi, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, 97074 Würzburg, Germany

Single particle manipulation offers unique possibilities to tune the electronic properties of molecular and atomic assemblies and thereby opens new pathways for future electronic devices. Therefore, the understanding of the underlying physical mechanisms is of significant importance. We have performed STM/STS measurements of single transition metal phthalocyanine (*TM*Pcs) molecules adsorbed on van der Waals surfaces. We find a voltage-dependent rotational movement threshold which coincidence with the energy of the lowest unoccupied molecular orbital (LUMO) [1] of the investigated molecules as determined by STS. Spatially resolved measurements reveal a good match between the spatial distribution of the rotational frequency and the LUMO conductance, indicating its strong involvement. We speculate that the rotational motion is, like in other molecules [2,3], a consequence of vibrational modes excited by the relaxation of electrons tunneling into the LUMO. Besides the acquisition of information correlated to the manipulation of *TM*Pc on van der Waals surfaces this technique provides an additional approach for energetically and spatially mapping the LUMO of rotationally unstable systems.

[1] A. Nickel *et al.*, ACS Nano **7**, 191 (2013).

[2] A. J. Mayne *et al.*, Chem. Rev. **106**, 4355 (2006).

[3] B. C. Stipe *et al.*, Phys. Rev. Lett. **81**, 1263 (1998).

O 63.5 Wed 16:45 H4

DFT Simulation of AFM-images of Fe, Cu and Si adatoms on Cu(111): different tip models — •Svitlana Polesya[1], Sergiy Mankovskyy[1], Hubert Ebert[1], and Franz Giessibl[2] — [1]Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München, Germany — [2]Institut für Experimentelle Phzsik, Univ. Regensburg, Germany

Atomic Force Microscopy (AFM) images for Fe, Cu and Si adatoms in there equilibrium positions on Cu(111) surface have been simulated on the basis of Density Functional Theory (DFT). We focus in the present work on the effect of different types of tips on the AFM image. For that reason, the forces experienced by the tip have been calculated for three tip models: single H atom, CO molecule and Cu_4 cluster. The calculated forces for the CO molecule tip fully reproduce the experimentally observed distance dependence of the force profile for a Cu adatom. Also the three fold symmetry of the lateral AFM-image for a Fe adatom, in contrast to a Cu adatom, can be explained using the results of the calculations. The nature of the repulsive forces at large lateral distances from the adatom position ($\sim$ 200-250 pm) is discussed on the basis of the electron density redistribution in the tip-adatom region.

O 64: Oxides and Interfaces: Adsorption II

Time: Wednesday 15:00–17:30 Location: H6

O 64.1 Wed 15:00 H6

Ab initio wave-function-based methods for highly accurate description of adsorption — •Denis Usvyat — Institut für Physikalische und Theoretische Chemie, Universtät Regensburg, 93040 Regensburg, Deutschland

The wave-function-based hierarchy of electronic structure models represents a convergent theory in a sense that it systematically approaches the exact solution within the Born-Oppenheimer approximation. Conventionally these models are computationally quite intensive and for decades were hardly applicable to extended systems. We show that by employing local approximations for the electronic correlations it becomes possible to overcome the issues of the computational complexity and treat periodic systems at a very high ab initio level. Furthermore, a combined periodic/finite-cluster approach allows one even to reach accuracy that surpasses the experimental one.

Physisorption on surfaces is one of the fields, where this technique is especially powerful. Indeed, the small energy scale and shallowness of the potential energy surfaces set high demands on the accuracy. On several examples we demonstrate that progressive elimination of various sources of errors, which is possible within the hierarchical wave-function-based treatment, leads to a sub-kJ/mol (or meV) accuracy in the interaction energies for small molecules adsorbed on non-conducting surfaces. Due to the unbiased character of this approach, it can be used to resolve experimental controversies, which are common in studies of physisorption.

O 64.2 Wed 15:15 H6

Effects of Flexibility and Entropy on the Adsorption and Growth of Functional Molecules — •David Gao[1], Julian Gaberle[1], Matthew Watkins[2], Filippo Federici Canova[3], Christian Loppacher[4], Laurent Nony[4], Ania Amrous[4], Franck Bocquet[4], Franck Para[4], and Alexander Shluger[1,5] — [1]University College London, London, UK — [2]University of Lincoln, Lincoln, UK — [3]Aalto University, Espoo, Finland — [4]Aix-Marseille University CNRS, Marseille, France — [5]WPI-AIMR Tohoku University, Sendai, Japan

In this work we combined noncontact atomic force microscopy (NCAFM) experiments and theoretical calculations to study the effects of molecular flexibility on the adsorption and self-assembly of organic molecules on KCl(001).

Rigid 1,3,5-tri-(4-cyano-4,4 biphenyl)-benzene (TCB) and flexible 1,4-bis(cyanophenyl)-2,5-bis(decyloxy)benzene (CDB) molecules were synthesized, deposited onto a KCl (110) surface, and imaged using NCAFM. Both molecules were observed to form ordered monolayer structures at room temperature. However, the dewetting properties and growth modes of these two molecules were qualitatively different. We performed density functional theory (DFT) and classical molecular dynamics (MD) calculations to consider both enthalpic and entropic contributions to adsorption energy. Our results show that entropic effects are significant for flexible molecules (such as CDB) and can have a pronounced effect on the mechanisms of self-assembly and structural stability.

O 64.3 Wed 15:30 H6

Copper deposition on stoichiometric and reduced ceria films — •Boris Gross and Niklas Nilius — Carl-von-Ossietzky Universität Oldenburg, Institut für Physik, D-26111 Oldenburg, Germany

Nearly stoichiometric and oxygen-deficient CeO_{2-x}(111) films, grown on Ru(0001), have been titrated with Cu nanoparticles in order to explore the interaction of noble metals with reducible oxides. In contrast to Ag and Au that preferentially bind along oxide step edges, Cu randomly nucleates even on mildly reduced ceria, as revealed from low-temperature STM measurements. The observed nucleation behavior indicates a considerable Cu interaction with O vacancies in the surface. Moreover, a distinct bimodal size distribution is revealed for the Cu particles, with the mean size substantially varying on adjacent and even on single oxide terraces. As recorded particle sizes display a strong dependence on the STM bias voltage used for imaging, an electronic origin for the bimodal size distribution is anticipated. We discuss self-limiting Cu growth as a result of charge-transfer from underlying Ce^{3+} ions as well as a variable O vacancy concentration in differently thick ceria patches as possible reasons for the observed effect.

O 64.4 Wed 15:45 H6

Exploring Pd adsorption, diffusion, permeation, and nucleation on bilayer SiO_2/Ru as a function of hydroxylation and precursor environment; from UHV to catalyst preparation — Sascha Pomp[1,2], William Kaden[2], •Martin Sterrer[1,2], and Hans-Joachim Freund[2] — [1]Institute of Physics, University of Graz, Graz, Austria — [2]Department of Chemical Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The hydroxylation-dependent permeability of bilayer SiO_2 supported on Ru(0001) was investigated by XPS and TDS studies. For this, the thermal behavior of Pd evaporated at 100 K, which results in surface and sub-surface binding arrangements, was examined relative to the extent of pre-hydroxylation. Samples containing only defect-mediated hydroxyls showed no effect on Pd diffusion through the film. If, instead, the concentration of strongly bound hydroxyl groups and associated weakly bound water molecules was enriched by an electron-assisted hydroxylation procedure, the probability for Pd diffusion through the film is decreased via pore-blocking. Above room temperature, all samples showed similar behavior, reflective of particle nucleation above the film. When depositing Pd onto the same SiO_2/Ru model-support via adsorption of $[Pd(NH_3)_4]Cl_2$ from alkaline (pH 12) precursor solution, we observe notably different adsorption and nucleation mechanisms. The Pd adsorption complexes follow established decomposition pathways to produce model-catalyst systems compatible with those created exclusively within UHV despite lacking the ability to penetrate the film due to the increased size of the initial Pd precursor groups.

O 64.5 Wed 16:00 H6

Single Rh adatoms at the Fe_3O_4(001) surface and their interaction with gas molecules — •Roland Bliem, Adam Zavodny, Michael Schmid, Peter Blaha, Ulrike Diebold, and Gareth Steven Parkinson — TU Wien, Vienna, Austria

Single-atom catalysis is a hot topic in catalysis research, aiming for high activity at optimum efficiency in the usage of precious metals. Understanding the reaction mechanisms in this emerging field requires atomic-scale information about the interaction of single metal adatoms with gas molecules. The Fe_3O_4(001) surface is an ideal model system to study adatom-gas interactions as well as a promising support material for single-atom catalysis, because its $(\sqrt{2}\times\sqrt{2})R45^\circ$ reconstruction [1] provides strong adsorption sites stabilizing single metal adatoms up to temperatures as high as 700K [2,3].

Here, we present a room-temperature study of Rh adatoms and their interaction with O_2, NO, CO, and H_2O using scanning tunnelling microscopy (STM) and density functional theory (DFT+U). Rh adatoms interact with each gas in a different way: O_2 adsorbs strongly, causing adatom mobility and sintering. NO adsorption also leads to mobility but hardly any clustering is observed. In contrast, CO adsorption does not induce mobility but poisons the activity for O_2 adsorption. Furthermore, Rh adatoms facilitate water splitting. DFT calculations yield bond strengths of O_2 and CO and metal-adsorbate bond lengths.

[1] Bliem et al. Science 346, 1215-1218 (2014).

[2] Novotny et al. Phys. Rev. Lett. 108, 216103 (2012).

[3] Bliem et al. ACS Nano 8, 7531-7537 (2014).

O 64.6 Wed 16:15 H6

N_2O to N_2 conversion on reduced ceria surface: NEXAFS and IRRAS studies — •Alexei Nefedov, Chengwu Yang, and Christof Wöll — Karlsruhe Institute of Technology, Karlsruhe, Germany

Ceria, one of the most reducible metal oxides, has proven to be a highly active catalyst for NO_x reduction to N_2. To monitor this conversion the NEXAFS and IRRA spectroscopies have been applied in a time-resolved fashion. The stoichiometric CeO_2 single crystals and powders were annealed at elevated temperatures in vacuum to create surface oxygen vacancies. N_2O exposure was achieved by backfilling up to 10^{-9} mbar at sample temperatures typically below 120 K. The NEXAFS measurements were carried out at the synchrotron facility BESSY II and for IRRAS experiments we used a novel UHV-IR spectrometer. In the NEXAFS spectra, two intense resonances (401.2 eV and 404.8 eV) with equal intensities are observed. These resonances decrease in parallel over time and this decrease is explained by conversion of N_2O to N_2 over reduced CeO_2. IRRAS data confirm NEXAFS results. After N_2O adsorption only one band at 2250 cm^{-1} is observed, which can be described as a nitrogen-nitrogen asymmetric stretching vibration. After the temperature increase as well as after the UV irradiation the band intensity goes down. Comparison of grazing emission XP spectra before and after N_2O treatment indicates N_2O donated oxygen atom to the oxygen vacancy and re-oxidized the reduced CeO_2.

O 64.7 Wed 16:30 H6

CO_2 and Water Adsorption on the $Fe_3O_4(001)$ Surface — •Jiri Pavelec, Jan Hulva, Roland Bliem, Oscar Gamba, Daniel Halwidl, Martin Setvin, Michael Schmid, Ulrike Diebold, and Gareth Parkinson — TU Wien, Vienna, Austria

The recently solved $Fe_3O_4(001)$ surface [1] is an exciting model system to investigate catalysis by supported single atoms [2] and sub-nano clusters [3]. However, understanding the interaction of the clean surface with the relevant molecules is an essential prerequisite to studying such composite systems.

Here we report a study of water and CO_2 adsorption using a new multi-technique vacuum system constructed at the TU Wien that combines molecular beam methods, UPS, XPS and TPD. Together with STM results these data are used to characterize the state of the molecules over a broad temperature range (50K - 600K).

CO_2 is physisorbed up to 115K, and desorbs with first-order kinetics from regular lattice sites. A small peak at 125K provides a quantitative measure of the surface defect concentration.

Water adsorbs molecularly at 100K, and most of the molecules in the first monolayer desorb in four peaks up to 250 K. Isotopic labelling suggest that the two smaller peaks at 320K and 520K are related to defects, the latter involving exchange of O with the surface.

[1] R. Bliem et al., Science 2014, doi:10.1126/science.1260556
[2] Parkinson et al., Nature Materials 2013, doi:10.1038/nmat3667
[3] R. Bliem et al., Angewandte Chemie 2015, doi:10.1002/anie.201507368

O 64.8 Wed 16:45 H6

On-surface generation and imaging of reactive intermediates by atomic force microscopy — •Niko Pavliček[1], Bruno Schuler[1], Sara Collazos[2], Nikolaj Moll[1], Dolores Pérez[2], Enrique Guitián[2], Gerhard Meyer[1], Diego Peña[2], and Leo Gross[1] — [1]IBM Research–Zurich, 8803 Rüschlikon, Switzerland — [2]CIQUS and Departamento de Química Orgánica, Universidade de Santiago de Compostela, Santiago de Compostela 15782, Spain

Atomic force microscopy with functionalized tips allows imaging of the chemical structure of surface-adsorbed molecules [1].

Recently, we applied this method to investigate arynes, a class of reactive intermediates, which are involved in many chemical transformations [2]. Usually, their characterization is a great challenge because of short lifetimes and high reactivities. Here, we demonstrate the generation and characterization of individual polycyclic aryne molecules on an ultrathin insulating film by means of combined low-temperature scanning tunneling and atomic force microscopy. We also show that the aryne reactivity is preserved at cryogenic temperatures.

[1] L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, Science 325, 1110 (2009).
[2] N. Pavliček, B. Schuler, S. Collazos, N. Moll, D. Pérez, E. Guitián, G. Meyer, D. Peña, and L. Gross, Nature Chem. 7, 623 (2015).

O 64.9 Wed 17:00 H6

CO adsorption on small Au_n (n = 1–4) structures supported on magnetite (111) surface — •Tomasz Pabisiak[1], Maciej J. Winiarski[1,2], and Adam Kiejna[1] — [1]Institute of Experimental Physics, University of Wrocław, Wrocław, Poland — [2]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland

The adsorption of CO on Au_n nanostructures (n = 1–4) formed on the Fe-terminated (111) surface of magnetite (Fe_3O_4) was studied using density functional theory in the generalized gradient approximation of Perdew-Burke-Ernzerhof form with Hubbard correction U, accounting for strong electron correlations. The structural, energetic, and electronic properties were examined for two classes of configurations of the adsorbed Au_n structures. The flattened ones of bilayer-like structure, were found energetically more favored than vertical ones. For both classes of structures the adsorption binding energy increases with the number of Au atoms in a gold structure. A detailed analysis of the bonding charge and of the electron charge rearrangements at the Au_n/oxide contacts is presented. It is found that the CO adsorption binding to the $Fe_3O_4(111)$ supported Au_n is up to twice as strong as to the bare magnetite surface. Analysis of charges on the atoms showed that in each case CO binds to the most positively charged (cationic) atom of the Au_n structure. Changes in the electronic structure of the Au_n species and of the oxide support are discussed.

This work was supported by the National Science Center (NCN), Poland, Grant No.2012/07/B/ST3/03009.

O 64.10 Wed 17:15 H6

The interaction of Li with thin layers of the ionic liquid [BMP][TFSA] adsorbed on rutile $TiO_2(110)$ and their thermal stability — •Benedikt Uhl[1,2], Maral Hekmatfar[1,2], Florian Buchner[1,2], and R. Jürgen Behm[1,2] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — [2]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89081 Ulm, Germany

Due to their low flammability the use of ionic liquids (IL) as component in Li ion battery electrolytes is one possibility for the development of safer battery systems. To gain a better understanding of the fundamental molecular processes at the electrode|electrolyte interface, the interaction of Li with thin layers of n-butyl-n-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide [BMP][TFSA] on rutile $TiO_2(110)$ was investigated by X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM) under UHV conditions. Even at 80 K, deposition of Li, either before or after [BMP][TFSA] deposition, leads to a reaction of Li with the TiO_2 substrate, forming Ti^{3+} species in the near surface region. Also the [BMP][TFSA] adlayers are partly decomposed in both cases, in the first case by reaction with the formed Ti^{3+} species, in the second case by direct reaction with adsorbed Li atoms. The decomposition products of [BMP][TFSA] agree with decomposition mechanisms calculated previously in literature.[1] The thermal stability of the resulting layers is monitored up to 630 K until complete decomposition of the adlayers. [1]M. C. Kroon, *Green Chem.* **2006**, *8*, *3*, 241; *Thermochim.Acta* **2007**, *465*, *1*, 40.

O 65: Organic Photovoltaics and Electronics

Time: Wednesday 14:45–18:30 Location: H2

Invited Talk O 65.1 Wed 14:45 H2

Ultrafast excitonic and charge transfer dynamics in nanostructured organic polymer materials — •Irene Burghardt[1], Robert Binder[1], Matthias Polkehn[1], and Hiroyuki Tamura[2] — [1]Institute for Physical and Theoretical Chemistry, Goethe University Frankfurt, Germany — [2]WPI-Advanced Institute for Material Research, Tohoku University, Japan

We present first-principles quantum dynamical studies of ultrafast photoinduced exciton migration and dissociation in functional organic materials, in view of understanding the key microscopic factors that lead to efficient charge generation in photovoltaics applications. The talk will specifically address (i) exciton dissociation and free-carrier generation in donor-acceptor materials, including models for P3HT-PCBM heterojunctions [1] as well as highly ordered thiophene-perylene diimide assemblies [2], (ii) exciton migration [3] and formation of charge-transfer excitons in oligothiophene H-aggregates, and (iii) exciton multiplication by singlet fission in acene materials [4]. Special emphasis is placed on the critical role of exciton and charge delocalization which are a sensitive function of molecular packing.

[1] H. Tamura, I. Burghardt, J. Am. Chem. Soc. 135, 16364 (2013), M. Huix-Rotllant, H. Tamura, I. Burghardt, J. Phys. Chem. Lett. 6, 1702 (2015). [2] T. Roland et al., Phys. Chem. Chem. Phys. 14, 273 (2012), J. Wenzel, A. Dreuw, I. Burghardt, Phys. Chem. Chem. Phys. 15, 11704 (2013). [3] J. Wahl, R. Binder, I. Burghardt, Comput. Theor. Chem. 1040, 167 (2014). [4] H. Tamura et al., Phys. Rev. Lett. 115, 107401 (2015).

O 65.2 Wed 15:15 H2

Non-Equilibrium Charge Carrier Dynamics in Organic Disordered Semiconductors — •Andreas Hofacker[1], Jan Oliver Oelerich[2], Alexey Nenashev[3], Florian Gebhard[2], and Sergei Baranovskii[2] — [1]Institute of Applied Photophysics, Dresden University of Technology, D-01069 Dresden — [2]Department of Physics and Materials Science Center, Philipps-University, D-35032 Marburg — [3]Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

Time-dependent processes in organic semiconductors dominated by non-equilibrium physics are subject of current debate in the scientific community. The understanding of these processes promises fundamental insights into transport and recombination dynamics of charge carriers in organic semiconductor devices such as organic solar cells, and can therefore reveal possibilities for further efficiency enhancement.

Based on an analytical model developed for inorganic disordered semiconductors by Orenstein and Kastner in 1981, we formulate a description of carrier thermalization and recombination in organic disordered semiconductors. For this purpose we extend the very transparent approach of Orenstein and Kastner to enable the description of low recombination rates and applicability of the approach to arbitrary density of tail states (DOS) functions. We predict that the behavior of systems with a Gaussian DOS, which organic semiconductors are commonly believed to be, is distinctively different from systems with an exponential DOS. This fact could be used to experimentally distinguish whether a given sample possesses an exponential or a Gaussian DOS by performing a time-dependent carrier density measurement.

O 65.3 Wed 15:30 H2

Mobility-limited recombination models for organic solar cells — •Alexander Wagenpfahl and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Recent results of kinetic Monte Carlo simulations indicate that recombination of charge carriers in organic semiconductor blends show a strong dependence on the domain size of neat material phases [1]. Consequently, the Langevin recombination model does not generally apply and has to be modified by the geometric mean of the charge carrier mobilities. Here, we present drift–diffusion simulations to reveal the influence of such a recombination model in comparison to the Langevin theory. We discuss differences in the quality of the solar cell current–voltage characteristics and distinguish the different processes which lead to a reduction of the observed recombination rate [2].

[1] Phys. Rev. Lett. 114, 136602 (2015)
[2] Phys. Rev. B 80, 075203 (2009)

O 65.4 Wed 15:45 H2

Energy-Gap Law of Non-Radiative Voltage Losses in Organic Solar Cells — •Johannes Benduhn[1], Kristofer Tvingstedt[2], Fortunato Piersimoni[3], Olaf Zeika[1], Donato Spoltore[1], Dieter Neher[3], and Koen Vandewal[1] — [1]IAPP, TU Dresden, Germany — [2]EP VI, Julius-Maximillian University of Würzburg, Germany — [3]IPA, University of Potsdam, Germany

The open-circuit voltage of organic solar cells is low as compared to their optical gap, indicating large energy losses per absorbed photon. These losses arise from the necessity of an electron transfer from an electron donor to an electron acceptor to dissociate the excitons, and furthermore from the recombination of the resulting free charge carriers. It has been shown that the energy loss in the electron transfer event can be below 0.1 eV, while radiative recombination losses are in principle unavoidable.

In this work, we investigate the remaining voltage losses due to non-radiative decay of charge carriers. We find that the non-radiative voltage losses increase when the energy difference between charge transfer (CT) state and ground state decreases. This behaviour is consistent with the "energy gap law for non-radiative transitions", which implies that internal conversion from CT state to ground state is facilitated by molecular vibrations. With this work, we identify a possibly intrinsic loss mechanism, which until now has not been thoroughly considered for organic photovoltaics, and which is different in its very nature as compared to the commonly considered inorganic photovoltaic loss mechanisms of defect, surface, and Auger recombination.

O 65.5 Wed 16:00 H2

Development of a photocapacitor based on printed solar cells and supercapacitors — •Katrin Anneser[1], Lukas Hörlin[2], Stephan Braxmeier[1], Andreas Baumann[1], Gudrun Reichenauer[1], and Vladimir Dyakonov[1,2] — [1]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg — [2]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

The main drawbacks of renewable energy sources such as wind and solar energy are unpredictable power fluctuations presenting a major challenge to stability and efficiency of the grid. With increasing fraction of these intermittent energy sources it is necessary to smooth the power before feeding it into the grid without just cutting off the fluctuations. We are following the few previous research activities aiming at combining a fast energy storage device, a supercapacitor, and a solar cell. Rather than developing a modular system our objective is an integrated layered system provided by printing the components from solution processed precursors. Those combined cells will provide a more constant power output compared to stand-alone photovoltaic systems and thus allow feeding into storage units with far slower kinetics (e.g. batteries) or the grid. We present the concept and the related boundary conditions and problems to be solved. Furthermore, we show experimental data from solar cells measured at a high frequency (every second) and derive the basic requirements in terms of power and energy density required for the storage unit per m^2 of the integrated system from these data.

O 65.6 Wed 16:15 H2

Passivation and modification of silicon nanowires towards hybrid solar cells — •Jessica Hänisch[1], Carola Klimm[1], Marc A. Gluba[1], Karsten Hinrichs[2], Iver Lauermann[3], Wolfram Calvet[3], Norbert H. Nickel[1], and Jörg Rappich[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Berlin, Germany — [2]ISAS e.V. - Leibniz-Institut für Analytische Wissenschaften, Berlin, Germany — [3]BESSY, Berlin, Germany

Hybrid solar cells combine inorganic and organic materials to benefit from both areas, particularly in terms of production costs and material consumption. The inorganic-organic interface needs to be well passivated, especially if nanowires with a high surface area are implemented to enhance light absorption. The silicon nanowires were prepared by metal assisted chemical etching (MACE). The etching procedure leads to surface damaging and thereby generates surface defects. These defects reside in the band gap and act as recombination centers. As a consequence, the amount of collected charge carriers is reduced and therefore, the power conversion efficiency decreases. We applied electropolishing procedures to the silicon surface to minimize the amount of surface defects. Changes in the density of surface defects were directly monitored by in-situ photoluminescence measurements. To preserve the improved surface passivation obtained after the electropolishing process we used (electro-)chemical grafting of small molecules and investigated the surfaces by infrared spectroscopy, x-ray photoelectron spectroscopy and photoluminescence measurements.

30 min. Coffee Break

O 65.7 Wed 17:00 H2

Vertical Organic Field-Effect Transistors - Functional Principles and Applications — •Alrun Aline Günther[1], Michael Sawatzki[1], Christoph Hossbach[2], Petr Formánek[3], Daniel Kasemann[1,4], Johannes Widmer[1], Johann W. Bartha[2], and Karl Leo[1,5] — [1]Institut für Angewandte Photophysik, TU Dresden, Germany — [2]Institut für Halbleiter- und Mikrosystemtechnik, TU

Dresden, Germany — [3]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [4]currently: CreaPhys GmbH, Dresden, Germany — [5]Fellow of the Canadian Institute for Advanced Research, Toronto (ON), Canada

Vertical organic field-effect transistors (VOFETs) are a means to overcome the limitations of conventional organic field-effect transistors (OFETs). At present however, they often suffer from two major drawbacks: performance limitation by contact effects and limitation to certain materials and processing techniques, making a controlled shift of parameters such as the transistor threshold voltage difficult. Here, we present p- and n-type VOFETs operating in the accumulation and inversion regimes. By introducing contact doping, we are able to increase the transconductance and On/Off ratio of VOFETs by an order of magnitude. We further show that the realisation of inversion VOFETs is possible and can shift the threshold voltage in a controlled manner, while reducing the Off state current of VOFETs through reduction of the source-drain leakage current.

O 65.8 Wed 17:15 H2

Vertical Organic Light Emitting Transistors for Investigation of Charge Transport in VOFETs

— •Franz Michael Sawatzki[1], Alrun Günther[1], Duyhai Doan[2], Christoph Hossbach[3], Petr Formánek[4], Daniel Kaseman[1,5], Johannes Widmer[1], Thomas Koprucki[2], and Karl Leo[1,6] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — [2]Weierstraß-Institut für Angewandte Analysis und Stochastik, Leibniz-Institut im Forschungsverbund Berlin e. V., Germany — [3]Institut für Halbleiter- und Mikrosystemtechnik, Technische Universität Dresden, Germany — [4]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [5]currently: CreaPhys GmbH, 01257 Dresden, Germany — [6]Fellow of the Canadian Institute for Advanced Research (CIFAR), Toronto, Ontario M5G 1Z8, Canada

The vertical organic field effect transistor (VOFET) offers many technological advantages due to its very short geometric channel length. However, in contrast to the standard lateral organic field effect transistor (OFET), the basic physics and working principles are not yet well known. Here, we compare results regarding the charge transport obtained from simulations with measured charge carrier density distributions. The latter ones are obtained from the light emission of vertical organic light emitting transistors (VOLETs). These devices are a combination of an organic light emitting diode (OLED) and a VOFET, which allow to locally resolve the current path. We show the dependence of the channel size and geometry on the gate-source voltage, the drain-source voltage, and the source geometry.

O 65.9 Wed 17:30 H2

Ultra-High Current Densities in Organic Transistors

— •Markus P. Klinger, Axel Fischer, Felix Kaschura, Daniel Kasemann, Johannes Widmer, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden

Organic transistors are considered for flat panel or flexible displays, radio identification systems, and sensor arrays. Much effort has been spent to optimize the charge carrier mobility and to reduce the channel length of organic field-effect transistors (OFETs). Likewise, new device concepts have been introduced based on charge transport perpendicular to the substrate utilized in so-called vertical organic transistors. One representative is the high-performing organic permeable-base transistor (OPBT) [1,2]. Here, we show that this device is determined by space-charge limited current (SCLC) in the on-state. Thus, OPBTs can drive as much current as possible for a certain thickness of semiconducting material. Using C_{60} with a low charge carrier mobility of about $0.025\,\mathrm{cm}^2\,\mathrm{V}^{-1}\mathrm{s}^{-1}$ in the vertical direction, current densities of more than $600\,\mathrm{A\,cm}^{-1}$ are reached at voltages below 6 V. This performance can be achieved as the total thickness of the device is in the range of 100 nm. With that, OPBTs can easily outperform OFETs in terms of current per footprint area.

[1] M. P. Klinger et al., Adv. Mater. (2015), 27(47);

[2] A. Fischer et al., Appl. Phys. Lett. (2012), 101, 213303

O 65.10 Wed 17:45 H2

Controlling the electronic properties in liquid crystal conjugated small molecules for application in electronics

— •Nadine Tchamba Yimga[1], Holger Borchert[1], Peer Kirsch[3], Jürgen Parisi[1], and Elizabeth von Hauff[2] — [1]Department of Physics, University of Oldenburg, Germany — [2]Department of Physics and Astronomy, VU University Amsterdam, The Netherlands — [3]Merck KGaA, Liquid Crystals R&D Chemistry, Germany

Organic semiconductors offer numerous advantages for electronics. However, carrier mobilities in organic semiconductors are generally orders of magnitude lower than in inorganic semiconductors. This is a major bottle neck for device efficiency. The electrical properties are additionally dependent on thin film morphology which is challenging to control in solution deposited films. We studied structure-function relationships in a novel liquid crystal molecule. The molecular films demonstrate phase changes from crystalline to nematic to isotropic phases at temperatures of 140 C, 165 C and 250 C, respectively. We demonstrate the influence of temperature on the structure of solution processed films with cross polarized microscope (CPM) and X-ray diffraction (XRD). Current-voltage measurements and impedance spectroscopy were performed on films annealed to temperatures above the crystalline - nematic phase change and subsequently cooled. The mobility increases from 10^{-4} cm^2 V^{-1} s^{-1} to 10^{-3} cm^2 V^{-1} s^{-1}. We demonstrate that controlled structural manipulation of the film can be used to reduce electronic disorder. These results show the potential of liquid crystal conjugated materials in electronic applications.

O 65.11 Wed 18:00 H2

Photodetectors Based on an Anilino Squaraine for Efficient Detection of Light in the 700 nm Region

— •Andre Pries[1], Matthias Schulz[2], Arne Lützen[2], Jürgen Parisi[1], and Manuela Schiek[1] — [1]Institute of Physics, Energy and Semiconductor Research Laboratory, Oldenburg, Carl von Ossietzky University, Germany — [2]Kekulé Institute of Organic Chemistry and Biochemistry, Bonn, Rheinische Friedrich-Wilhelms-University, Germany

In this work the squaraine derivative 2,4-bis[4-(N,N-diisobutylamino)-2,6-dihydroxyphenyl] squaraine (SQIB) is analyzed in a conventional bulk-heterojunction photodiode architecture, Glass/ITO/MoO_3/SQIB:PCBM/LiF/Al. This architecture shows a power conversion efficiency of ≈2.5 % and a peak external quantum efficiency (EQE) of ≈50 % at 700 nm, making the device highly sensitive in the red wavelength region. In order to even further increase the EQE a negative bias voltage is used. Next the time-dependent response of the device is measured, to find, e.g. the rise- and fall time. Finally, the bandwidth of the device is determined and the cut-off frequency.

[1] G. Chen et. Al, Optical and electrical properties of a squaraine dye in photovoltaic cells, Applied Physics Letters, Vol. 101, No.8 2012, 083904

[2] M.Binda et. Al, Fast and air stable near-infrared organic detector based on squaraine dyes, Organic Electronics, 2009, Vol. 10, Issue 7, p. 1314-1319

O 65.12 Wed 18:15 H2

First results of an implementation of GW of reduced complexity for organic semiconductors

— •Saber Gueddida and Dietrich Foerster — LOMA, Université de Bordeaux, France

We have implemented a GW algorithm of reduced complexity (N^3 rather than N^4) for crystals containing N»1 atoms in their unit cell. The main ideas of the algorithm and first results of its implementation will be given. Our code aims at contributing to optimizing organic solar cells by predicting the bands and gaps of their constituents.

O 66: Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Time: Wednesday 18:15–20:30 Location: Poster A

O 66.1 Wed 18:15 Poster A

Improving anharmonic vibrational calculations from first principles — •Joseph C.A. Prentice, Bartomeu Monserrat, and Richard J. Needs — TCM Group, Cavendish Laboratory, University of Cambridge, UK

The vibrational self-consistent field (VSCF) method, as described in PRB 87 144302, has had several successes in accurately calculating the anharmonic properties of various materials, such as diamond, ice and solid hydrogen. However, a practical issue with the method is the large number of DFT calculations required to map the Born-Oppenheimer energy surface sufficiently accurately. We look at improvements to the method that reduce this computational load, in particular using data on forces from DFT calculations to improve the accuracy of the mapping. Results using this improved method are presented for competing structures of silicate perovskite under lower mantle conditions. Further improvements, involving the inclusion of n-body coupling between phonons, and their possible implementation are also discussed.

O 66.2 Wed 18:15 Poster A

Towards a practical implementation of second-order Møller-Plesset perturbation theory for solids — •Xiangyue Liu, Arvid Conrad Ihrig, Sergey Levchenko, Igor Ying Zhang, and Matthias Scheffler — *Fritz-Haber-Institut der MPG, Berlin, DE*

The second-order Møller-Plesset perturbation theory (MP2) method is gaining attention in materials science, because it is free from the one-electron self-interaction error. Such error, as a lasting problem in density-functional theory, can lead to a wrong prediction of electronic band gaps, charge transfers, and reaction barriers, all of which are ubiquitous electronic properties or behaviors in condensed-matter systems. However, the unfavourable computational complexity, especially the cubic scaling with respect to the $\boldsymbol{k}$-point number in reciprocal space, limits the applicability of MP2 for solids. In this project we present a practical MP2 implementation for solids in the all-electron full-potential framework. In our implementation, the MP2 correlation energy is evaluated in the atomic-orbital (AO) representation (AO-MP2), which allows for a lower computational scaling in both real and reciprocal spaces[1]. The localized resolution of identity (RI-LVL) technique[2] is adopted to address the memory bottleneck of the AO-MP2 method, making it feasible to handle systems with several hundred atoms per supercell while avoiding the reliance on the disk storage. We demonstrate the accuracy as well as the efficiency of our new MP2 implementation for a diverse set of materials. [1] Levchenko, S. V. *et al.*, Comput. Phys. Comm. **192**, 60, (2015); [2] Ihrig, A.C. *et al.*, New J. Phys. **17** 093020, (2015).

O 66.3 Wed 18:15 Poster A

Application of the exact exchange functional to magnetic metals within the FLAPW method — •Max Nusspickel[1], Markus Betzinger[1], Christoph Friedrich[1], Andreas Görling[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Orbital-dependent functionals form a promising class of exchange-correlation (xc) functionals in Kohn-Sham density-functional theory. Already the simplest functional of its kind, the exact exchange functional (EXX), cures the unphysical Coulomb self-interaction error of LDA and GGA functionals. In order to obtain a local xc potential from an orbital-dependent functional, the optimized effective potential (OEP) method is used, resulting in an integral equation for the potential. This equation, however, determines the potential only up to a constant.

In spin-polarized metals, the alignment of the spin-up and spin-down potentials is obtained by the requirement of electron number conservation: variations of the potential can lead to a change of the Fermi energy and, hence, to a variation of the densities of both electron spins. In this way, the OEP equations for the spin-up and spin-down potentials are coupled and the spin-dependent xc potential is obtained from a single OEP equation. We discuss the extension of our EXX-OEP implementation within the linearized augmented plane-wave (FLAPW) method and show results for prototype magnetic metals.

O 66.4 Wed 18:15 Poster A

Electric switchable giant Rashba-type spin splitting in bulk PbS — •Bin Shao[1], Wenhui Duan[2], and Thomas Frauenheim[1] — [1]BCCMS, University of Bremen, Bremen, Germany — [2]Institute for Advanced Study, Tsinghua University, Beijing, China

Realizing electric controllable spin is one of the major challenges in the field of spintronics. A promising approach is to utilize so-called Rashba effect, which arises from the spin-orbit coupling under broken inversion symmetry, leading to a momentum-dependent spin splitting in k-space. However, the sizes of this splitting are usually rather small, which hinders the application of this effect in spintronics. In this work, based on density functional calculation, we predict a giant Rashba-type spin splitting in bulk PbS with space group $P6_3mc$. The phonon spectrum calculation gives evidence of the thermal stability of this system. The origin of the giant Rashba effect has been demonstrated from the deviation of the S ion from the inversion symmetric position, leading to an ferroelectric polarization along c axis. By switching the direction of the ferroelectric polarization, the spin directions of bulk carriers governed by the Rashba effect are completely rotated, which grants a potential approach to manipulate the spin of electrons by an external electric field. Moreover, under a reasonable hydrostatic pressure, the system could obtain the inversion symmetry due to the movement of the S ion backwards to symmetric positions. As a result, the system turns into a topological phase with the massless Dirac cone state at the (001) surface.

O 66.5 Wed 18:15 Poster A

GW+fRG: Towards an fRG enhancement of ab initio calculations — Jannis Ehrlich[1,2], Carsten Honerkamp[1], Christoph Friedrich[2], and •Stephan Blügel[2] — [1]Institut für theoretische Festkörperphysik, RWTH Aachen University, D-52056 Aachen, Germany — [2]PGI-1 and IAS-1, FZJ & JARA, D-52425 Jülich, Germany

Spin excitations in solids are of fundamental interest for a wide variety of phenomena. Most materials-specific theoretical studies are based on the adiabatic treatment of the spin-degees of freedom in the context of DFT. Approaches based on the *GW* approximation include screening effects due to charge fluctuations but neglect vertex corrections and other contributions like magnetic fluctuations. The functional renormalization group (fRG) can overcome these limitations as it resums a different class of diagrams, among them charge and magnetic fluctuations and vertex corrections. We discuss how the equations for two-particle vertices in the fRG contain the *GW* approximation, the Bethe-Salpeter equation (BSE) and the parquet approach on certain levels of approximations. Thus, a fRG calculation of materials properties could be a powerful approach to improve the *GW* and BSE methods already applied in first-principles calculations. By using recently suggested channel decomposition schemes [1,2] the method has gained in flexibility and in potential for tackling more complex tasks. Here we propose first steps to develop the fRG approach for the *ab initio* calculation of materials properties.

[1] C. Husemann, M. Salmhofer, Phys. Rev. B **79**, 195125 (2009).

[2] W. Wang *et al.*, Phys. Rev. B **85**, 035414 (2012).

O 66.6 Wed 18:15 Poster A

The quantum anomalous Hall effect in HgMnTe — •Jan Böttcher, Christoph Kleiner, and Ewelina M. Hankiewicz — Uni Würzburg, Institut für Theoretische Physik und Astrophysik, Germany

Recently, the quantum anomalous Hall (QAH) effect was predicted to exist in Mn doped HgTe. Within the QAH phase only one edge state remains at an edge due to an opposite coupling of spin to the magnetization. The experimental proof is however still outstanding. The paramagnetic nature of the Mn impurities gives rise to the formation of Landau levels which makes it experimentally challenging to distinguish the QAH from a conventional quantum Hall (QH) state. Based on the BHZ model, we present an extended study of the transition from the quantum spin Hall to the QAH state as well as the QAH to the quantum Hall state. For this purpose, we make use of the finite difference method and compare the results with analytical calculations. Hallmarks of the QAH states in the presence of magnetic fields are discussed. The BHZ model has natural limitations in the high magnetic field regime. We therefore compare our results with band structure calculations based on the 8x8 Kane Hamiltonian. Signatures in the magnetoresistance are discussed which might open the door to distinguish the QAH from the QH state in future transport experiments.

We acknowledge financial support by the DFG within SFB 1170 "ToCoTronics".

O 66.7 Wed 18:15 Poster A

Nonconventional screening of the Coulomb interaction in low-dimensional semiconductors and insulators — Ersoy Sasioglu, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Screening effects play a fundamental role in determining the exciton binding energy, electron dynamics, and the effective electron-electron interaction in low-dimensional semiconductors and insulators. Experimental observation of the large exciton binding energies and nonhydrogenic Rydberg series in low-dimensional semiconductors indicate an unusual non-local screening of the Coulomb interaction. By means of first-principles calculations in conjunction with the random-phase approximation (RPA) within the FLAPW method we study the screening of the Coulomb interaction in low-dimensional semiconductors and insulators. For this purpose a novel tetrahedron method has been implemented. We show that the screening in these systems deviates substantially from the bulk behavior, i.e., the screened interaction W cannot be expressed by a simple static dielectric constant. We compare the numerical RPA results to analytical functions derived from image-charge models for the isolated slab and for a repeated slab model. We find a nonconventional screening in low-dimensions. This nonconventional screening explains the deviations from the usual hydrogenic Rydberg series of energy levels of the excitonic states in one- and two-dimensional semiconductors and opens up possibilities for fundamental studies of correlation effects in low-dimensional materials.

O 67: Theory: General

Time: Wednesday 18:15–20:30 Location: Poster A

O 67.1 Wed 18:15 Poster A

Excited-state lifetimes in binuclear copper centers calculated from first principles — •Martin Rohrmüller[1], Maria Naumova[1,2], Michael Rübhausen[2], Gerald Henkel[1], and Wolf Gero Schmidt[1] — [1]Universität Paderborn, 33098 Paderborn, Germany — [2]Universität Hamburg, 20355 Hamburg, Germany

Proteins containing copper sulfur complexes play a key role for electron transfer in biological systems. In order to explore the interplay between the structural and electronic degrees of freedom in these systems, smaller biomimetic model complexes such as $[Cu_2((NGuaS\text{-})_2)_2]^{2+}$ [1] are investigated.

In this presentation we explore the electronic structure and in particular the lifetime of electronic excitations in $[Cu_2((NGuaS\text{-})_2)_2]^{2+}$. To that end the imaginary parts of the electron self-energies – related to the quasi-particle lifetime due to electron-electron interaction – are calculated within many-body perturbation theory based on the density functional theory electronic structure [2].

We analyze the metal to ligand charge transfer (MLCT) excitations of the model complex including structural relaxations and discuss in detail the numerical stability and convergence of the calculated electronic self-energy with respect to the simulation parameters.

[1] A. Neuba *et al.* Angew. Chem. Int. Ed., **51**, 1714 (2012).

[2] A. Marini *et al.* Phys Rev. B **66**, 161104R (2002).

O 67.2 Wed 18:15 Poster A

Interplay of structural and electronic properties in thin-film absorbers — •Thomas Bischoff[1], Claudia Schnohr[2], and Silvana Botti[1] — [1]Institut für Festkörpertheorie und theoretische Optik, 07743 Jena, Germany — [2]Institut für Festkörperphysik, 07743 Jena, Germany

During the past years, $Cu(In,Ga)(Se,S)_2$ (CIGS) thin-film solar cells have emerged as a technology that could challenge the current hegemony of silicon solar panels. CIGS compounds conserve to a very high degree their electronic properties in a large non-stoichiometric range and are remarkably insensitive to radiation damage or impurities. The family of kesterites $Cu_2ZnSe(S,Se)_4$ (CZTS) exhibits very similar electronic properties. Moreover, kesterites have the clear advantage of being composed of abundant, non-toxic, less expensive chemical elements. However, the efficiency of CZTS solar cells is about 50% smaller than the one of CIGS solar cells.

The origin of the exceptional electronic properties and the defect physics of these compounds and their alloys is still far from being completely understood, despite the large amount of experimental and theoretical work dedicated to that purpose.

We present here self-consistent GW calculations of the dependence of the band gap on internal distortions. Combined with EXAFS measurements, our calculations allow to quantify the structural contributions to the band gap bowing of alloys of these families.

O 67.3 Wed 18:15 Poster A

Efficient Moller-Plesset perturbation theory for extended systems — •Theodoros Tsatsoulis and Andreas Grüneis — Max-Planck-Institute for Solid State Research, Stuttgart

Kohn-Sham density functional theory is one of the most popular methods used in material science. However, many functionals cannot accurately determine the energetics of solids and surfaces. Furthermore, there is no systematic way to improve upon the functionals. The wave-function based treatment of electronic correlation constitutes a hierarchy of methods that allows one to systematically approximate the many-body nature of the true ground state wave-function, however, with a large computational cost. The latter stems to a large extent from the unfavorable scaling of the computational cost with the number of virtual states. It is therefore critical to span only the relevant parts of the virtual space for the implementation of efficient wave-function based methods. We consider an approach whereby the occupied orbitals are converged in a plane wave basis, whereas the virtual space is then constructed using pseudized Gaussian orbitals expanded in plane waves. This approach allows for an efficient implementation of wave-function based methods. Results are shown for water adsorption on surfaces at the level of Møller-Plesset perturbation theory within the projector-augmented-wave method as implemented in VASP [1].

[1] Marsman et al., The Journal of Chemical Physics, 130, 184103 (2009)

O 67.4 Wed 18:15 Poster A

Implementation of electron-phonon coupling in the KKR formalism — •Carsten Eberhard Mahr, Michael Czerner, Christian Franz, and Christian Heiliger — Justus-Liebig-University, Giessen, Germany

Electron-phonon coupling is one of the main incoherent inelastic scattering mechanisms in a wide variety of crystalline material systems at room temperature. Therefore, it is necessary to incorporate those effects in any realistic calculation of thermoelectric properties. We do so by extending our density functional theory (DFT) based Korringa-Kohn-Rostocker (KKR) Green's function formalism code.

By approximating the Fröhlich-type interaction with a self-energy $\Sigma_{\text{eph}} = -i\frac{\hbar}{2\tau}$ we can compute the dressed propagator G by solving Dyson's equation $G = G_{\text{ref}} + G_{\text{ref}} \cdot \left(\Delta V + \Sigma_{\text{eph}}\right) \cdot G$, where G_{ref} is an arbitrary (though typically repulsive) reference system. The electron-phonon scattering time τ may be extracted from e.g. electron linewidth calculations.

We present mathematical and implementational details of the beforementioned calculational scheme for non-equilibrium properties in the KKR basis set and discuss it's physical validity by evaluating resistivity characteristics of simple transport systems.

O 67.5 Wed 18:15 Poster A

Deblurring of Photoelectron Diffraction (XPD) Signals — •Christopher Kohlmann, Tobias Lühr, Christoph Keutner, Dominique Krull, and Carsten Westphal — Experimentelle Physik I, TU Dormtund, Germany, Otto-Hahn-Str. 4, 44221 Dormtund

The photoelectron diffraction (XPD) is a established and appropriate method for the analysis of the structure of surface and interfaces.

In order to regain the structural information out of the experimental data, simulations have to be performed. Precise reconstruction of the atomic structure can be determined by comparing the experimental and simulated data. We use a self made automated genetic algorithm to gain a better performance in quantity and quality. In order to reduce the influence of experimental artefacts, we are going to perform deblurring procedures on the experimental patterns. Therefore, the kernel function and the real diffraction effects of the sample need to be deconvoluted. Hence, the kernel function as well as a suitable data sampling method have to be found. This deconvolution method can also be applied on other experimental methods, like STM and PEEM.

O 68: Nanostructures at Surfaces: 1D, 2D Structures and Networks

Time: Wednesday 18:15–20:30 Location: Poster A

O 68.1 Wed 18:15 Poster A

Electronic structure of semiconductor superlattices — •Marlou Slot[1], Jaco Geuchies[1], Joep Peters[1], Efterpi Kalesaki[2,3], Christophe Delerue[3], Ingmar Swart[1], and Daniel Vanmaekelbergh[1] — [1]Condensed Matter and Interfaces, Utrecht University, Utrecht, the Netherlands — [2]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg, Luxembourg — [3]IEMN - Département ISEN, UMR CNRS 8520, Lille, France

In the search for materials for (opto-)electronic applications, two-dimensional metal chalcogenide semiconductors have emerged as high-potential candidates. In addition to the atomic structure, the nanoscale lattice of the material has a significant influence on the electronic band structure. Oriented attachment of colloidal nanocrystals results in atomically coherent semiconductor superlattices with a long-range square or honeycomb periodicity. [1] Tight-binding calculations predict a rich electronic structure that is determined by strong electronic coupling between the periodically arranged nanocrystals. [2,3] Using scanning tunneling spectroscopy, we studied the local density of states of the superlattices.

1. W.H. Evers et al., Nano Lett. 13, 2317 (2013).
2. E. Kalesaki et al., Phys. Rev. B 88, 115431 (2013).
3. E. Kalesaki et al., Phys. Rev. X 4, 011010 (2014).

O 68.2 Wed 18:15 Poster A

Structure of Cu(100)-c(2x2)N surfaces — •Julia Andrews, Kariman Elshimi, Torsten Veltum, and Mathias Getzlaff — Institut für angewandte Physik, Universität Düsseldorf, 40225 Düsseldorf

Nanostructured surfaces have become of significant interest in the field of surface science over recent years. The understanding of self-arranged structures is relevant for instance for the use as a pattern for nanoparticle deposition. We study the pattern that nitrogen forms when reacting with a Cu(100) surface.

Under ultra-high vacuum conditions, we first proceed to a standard cleaning of the copper crystal by sputtering with argon followed by annealing. To prepare the Cu(100)-c(2×2)N surface we sputter with activated nitrogen followed again by annealing.

We examine the crystal structure by low energy electron diffraction (LEED). With a scanning tunnelling microscope (STM) we observe how the nitrogen arranges itself when forming $\mathrm{Cu}_x\mathrm{N}$.

O 68.3 Wed 18:15 Poster A

Sierpiński-triangle fractal crystals with the C3v point group — •Daoliang Song[1] and Yongfeng Wang[1,2] — [1]Key Laboratory for the Physics and Chemistry of Nanodevices, Peking University, Beijing 100871, China — [2]Beida Information Research (BIR), Tianjin 300457, China

Self-similar fractals exist widely in nature, from the well-known snowflakes to the complicate Saturn's rings and are not only fundamentally important in both science and engineering, but also interesting in esthetics. Metal-organic Sierpiński triangles are particularly attractive for applications in gas separation, catalysis and sensing. Such fractals are constructed in this study by using 120°V-shaped 4,4"-dicyano-1,1':3',1"-terphenyl molecules and Fe atoms on Au(111), and studied in detail by low-temperature scanning tunneling microscopy. Density functional theory calculations are employed to rationalize the invisible Fe atoms in STM images. Monte Carlo simulations are performed to understand the formation mechanism of the surface-supported fractal crystals.

O 68.4 Wed 18:15 Poster A

Glancing angle deposition of metals — •Susann Liedtke, Christoph Grüner, Jürgen W. Gerlach, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig, Germany

Glancing angle deposition (GLAD) represents an ultrahigh vacuum physical vapor deposition process that utilizes self-shadowing of growing crystallites. Such self-shadowing effects occur if the substrate is strongly tilted with respect to the incoming particle flux. So far, the growth of metallic GLAD nanostructures remains poorly understood. For that reason, in this study GLAD of metals with different melting points is examined. Precisely, Ti and Al nanostructures are grown on unstructured Si substrates. The growth of metal nanostructures is investigated depending on process parameters such as substrate temperature and the incidence angle of the particle beam. Finally, the resulting nanostructures are compared with each other.

O 68.5 Wed 18:15 Poster A

Electromigration to create nanoscale gaps for molecular electronics — •Atasi Chatterjee, Frederik Edler, Christoph Tegenkamp, and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik, 30167, Hannover, Germany

The fundamental size limitations of today's silicon based technologies can be solved by the bottom up approach,if stable and reproducible nanometer spaced electrodes can be generated, and single (organic) molecules can be reproducibly attached to them in well-defined geometries. Therefore,fabrication of reliable contacts in order to investigate the functionalities of the molecules is a primary challenge. Electromigration, which was earlier well known as a failure mechanism of integrated circuit metallizations subjected to high current densities, now serves as one of the most promising methods of fabricating metallic nanogaps. We create flat ultrathin silver nanocontacts at the centre via electro-migration of lithographically prepared silver nanowires on a silicon substrate. A thin adhesion layer of Cr is used for Ag contact pads to avoid contact problems with STM tips. Electromigration is performed in a 4-tip SEM/STM chamber where two tips are used to contact the structure and a software controlled process is used to reach the tunneling regime at a preset tunneling resistance.Ultrathin and laterally open contact structures allow direct access for the STM tips for local control, in-situ observation and characterization of the gap. By detailed investigations of the dependence on current density and temperature, we try to explore the underlying physical mechanisms that form electromigrated gaps.

O 68.6 Wed 18:15 Poster A

ARPES Studies of the Bi/InAs(100) Interface — Olivier Heckmann[1,2], •Maria Christine Richter[1,2], Uros Djukic[1], Weiming Wang[3], Ivana Vobornik[4], Jean-Michel Mariot[5], Jan Minar[6,7], Jürgen Braun[6], Hubert Ebert[6], and Karol Hricovini[1,2] — [1]LPMS, Université de Cergy-Pontoise, Cergy-Pontoise, France — [2]DSM/IRAMIS/SPEC, CEA Saclay, Gif-sur-Yvette, France — [3]Tongji University, Shanghai 200092, China — [4]APE beamline, Sincrotrone Trieste, Area Science Park, Basovizza, Italy — [5]LCP-MR, Université P et M Curie/CNRS, Paris, France — [6]LMU Munich, Munich, Germany — [7]University of West Bohemia, Czech Republic

In this contribution we present ARPES studies of Bi/InAs(100) interface. Bismuth deposition followed by annealing of the surface results in the formation of one full Bi monolayer decorated by Bi-nanolines. We found that the building up of the interface does affect the electronic structure of the substrate. As a consequence of weak interaction, bismuth states are placed in the gaps of the electronic structure of InAs(100). We observe a strong resonance of the Bi electronic states close to the Fermi level; its intensity depends on the photon energy and the photon polarization. These states show nearly no dispersion when measured perpendicular to the nanolines, confirming their one-dimensionality. Interestingly, Bi atoms behave as donors, as their presence results in the appearance of an accumulation layer.

O 68.7 Wed 18:15 Poster A

Heat-induced formation of 1D and 2D coordination polymers on Au(111) — Tuan Anh Pham[1], Fei Song[1], Mariza N. Alberti[2], Manh-Thuong Nguyen[3], Carlo Thilgen[2], Francois Diederich[2], and •Meike Stöhr[1] — [1]University of Groningen — [2]ETH Zürich — [3]International Centre for Theoretical Physics, Trieste

In the fast growing research field of on-surface molecular self-assembly, coordination bonding is considered as an important tool for the construction of low-dimensional molecular networks on metal surfaces. To date, most of the reported metal-ligand coordination units are based on the combination of organic ligands bearing pyridyl, cyano, hydroxyl or carboxyl endgroups and transition-metal atoms such as Cu, Fe, Co or Ni. However, the construction of such MOFs on Au surfaces with native Au atoms is hardly reported. Here, we show that MOFs comprising porphyrin derivatives can be formed on Au(111) upon annealing. Both a threefold and a fourfold coordination motif stabilizing the MOFs were found. These findings were compared to MOFs made from the same porphyrin derivatives and Co atoms. For this, Co atoms and porphyrin derivatives were deposited on Au(111).[1] In both cases, the same structures were observed what evidences that indeed a coordination bonding is formed between the cyano groups and gold atoms. Moreover, we also investigated the influence of the position of the substituents (cis- vs. trans-isomers) on the MOF formation on Au(111). We could successfully demonstrate that the dimensionality of the MOF can be tuned from 1D to 2D depending on the chosen isomer.

[1] T.A. Pham et al., Chem. Commun. 51 (2015) 14473

O 68.8 Wed 18:15 Poster A

Tuning the Interaction of Magnetic Molecules with a Metallic Substrate via an Insulating Film — David Schwickert[1], Maciej Bazarnik[1], •Micha Elsebach[1], Bernhard Bugenhagen[2], Marc H. Prosenc[3], and Roland Wiesendanger[1] — [1]Institute for Nanostructures and Solid State Physics, University of Hamburg, D-20355 Hamburg, Germany — [2]Institute of Inorganic Chemistry, University of Hamburg, D-20146 University of Hamburg, Germany — [3]Dept. of Chemistry, Technical University Kaiserslautern, Erwin-Schrödinger-Str. 52, D-67663 Kaiserslautern, Germany

Magnetic molecules are a promising approach towards spin-based information technology. We use Co-Salophene as a tailored building block for spintronic devices. The possibility to build self-assembled covalently bonded chains by tailored on-surface chemistry makes this molecule a perfect candidate for an all-spin based device.

However, it is necessary to eliminate Kondo screening of the magnetic centers of the molecules. We use ultrathin films of NaCl to decouple the molecules from the metallic surface. The Ullmann reaction requires a Au-crystal as catalyst. Therefore, we intercalate the presynthesized chains with NaCl.

In this presentation we show the dependence of the intercalation on the sample temperature during the deposition, as well as the deposition rate and time. For low coverages of NaCl, monolayer and double layer islands grow between the chains. With increasing coverage the chains are pushed ahead by the growing islands. When two islands grow together, a chain lying between them is lifted up.

O 68.9 Wed 18:15 Poster A

Self-assembly and stability of bridged triphenylamine derivatives on metal surfaces — •Christian Steiner[1], Ute Meinhardt[2], Bettina Gliemann[2], Martin Gurrath[3], Bernd Meyer[3], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, FAU Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg, Germany — [3]Computer-Chemie-Centrum, FAU Erlangen-Nürnberg, Germany

Molecular self-assembly is a key concept in supramolecular chemistry and nanoscience allowing for the construction of complex molecular architectures in a bottom-up approach through noncovalent interactions. The adsorption, chemical nature, and self-assembly of diaminotriazinyl- and carboxyl-substituted triphenylamines with dimethylmethylene bridges were studied on Au(111) and Cu(111) at submonolayer coverage by low-temperature scanning tunneling microscopy and density functional theory calculations.[1] While the self-assemblies on Au(111) are strongly directed by intermolecular hydrogen bond interactions, on Cu(111) both molecules aggregate in dense islands owing to the stronger molecule-surface interaction. The carboxyl substituents partially deprotonate at room temperature on Cu(111). The diaminotriazinyl-substituted triphenylamines adsorb mainly intact at room temperature and deprotonate gradually at increased adsorption temperatures changing the bonding mechanism from hydrogen bonding to metal-ligand interactions.

[1] C. Steiner et al. J. Phys. Chem. C, 119 (46), 25945-25955 (2015)

O 68.10 Wed 18:15 Poster A

Growth competition between Sierpiński triangle fractals and two-dimensional molecular crystals of H3PH on noble metal surfaces — •Xue Zhang[1] and Yongfeng Wang[1,2] — [1]Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing, China — [2]Beida Information Research (BIR), Tianjin, China

Recent studies demonstrate that simple functional molecules, which usually form 2D crystal structures when adsorbed on solid substrates, are also able to self-assembly into ordered openwork fractal aggregates. To direct and control growth of such fractal supramolecules it is necessary to explore the conditions under which both fractal and crystalline patterns develop and coexists. In this contribution, we study the coexistence of Sierpińnski triangle (ST) fractals and 2D molecular crystals which were obtained by adsorption of H3PH molecules on Au(111) in high vacuum. Growth competition between the STs and 2D crystals was realized by tuning surface coverage as well as by changing the substrate and functional groups of the molecular building block. To better understand the mechanisms of the fractal structure formation our experimental studies were accompanied by theoretical calculations with Density Functional Theory and Monte Carlo methods. The obtained results demonstrate the possibility of steering the self-assembly to create surface-supported fractal and non-fractal structures made up of the same material.

O 68.11 Wed 18:15 Poster A

Analysis of structural and mechanical properties of long chain self-assembled monolayer on Au(111) by STM and AFM — •Torben Marx, Dirk Dietzel und André Schirmeisen — Institut für Angewandte Physik, Justus-Liebig-Universität, Gießen

Self-assembled monolayers (SAMs) are considered potential building blocks for a variety of nanotechnology applications. They are employed in e.g. the fields of material protection, electrode modification in electrochemistry, lithography as well as biology and medicine. The specific structural and mechanical properties of SAMs are the result of a spontaneous formation of organized objects out of smaller units, i.e. molecules, and are typically of crucial importance for any application. An important parameter in this context is the chain length of the molecules. Short-chain alkanethiol SAM on Au(111) are well studied and it was found that at saturation coverage the monolayer is typically of complex structure. In this work we have analyzed a long-chain alkanethiol (hexadecanethiol), which have been rarely studied up to now due to their relatively high resistance in STM. We found distinct orientated domains with the typical ($\sqrt{3}$x$\sqrt{3}$)R30° structure to exist. The adsorbate was structured further into a c(4x2) superlattice, which splits up in five different phases [1]. Additionally we have used AFM to analyze the mechanical properties of SAM with respect to stability and self healing capabilities.

[1] Lüssem et. al.,Langmuir , 21, 5256-5258 (2005)

O 68.12 Wed 18:15 Poster A

Metal-Peptide Coordination Complexes on Surfaces by Electrospray Ion Beam Deposition — •Elise Duquesne[1], Sabine Abb[1], Ludger Harnau[1], Stefan Rauschenbach[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Peptides are flexible biopolymers of a unique sequence of amino acids, which defines intramolecular interactions. In metal-peptide coordination complexes, the type of metal and its specific interaction with the peptide influences the coordination site and thus has an impact on the conformation of the peptide. Generally biomolecules cannot be evaporated due to their thermal instability, however by adding a metal salt to an electrospray solution of peptides a beam of well-defined coordination complexes can be readily formed and mass-filtered to select the coordination complex of interest. The aim of our study is to investigate the structures of metal-peptide complexes deposited on an atomically defined surface in ultra-high vacuum and to compare them with pure peptide structures [1]. Our work paves the way towards rational design of surface supported coordination complexes that can be relevant for a great number of applications in particular biomimetic catalysis.

References : [1] S. Abb, L. Harnau, R. Gutzler, S. Rauschenbach, K. Kern, Two-dimensional honeycomb network through sequence-controlled selfassembly of oligopeptides, Nature Communication, Accepted.

O 68.13 Wed 18:15 Poster A

Pyrazine as a Directing Group in Control of Reactivity and Regioselectivity for On-Surface Dehydrogenative Aryl-Aryl Bond Formation — •Nemanja Kocić[1], Xunshan Liu[2], Songjie Chen[2], Silvio Decurtins[2], Jascha Repp[1], and Shi-Xia Liu[2] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Department of Chemistry and Biochemistry, University of Bern, 3012 Bern, Switzerland

Regioselectivity is of fundamental importance in chemical synthesis. While many concepts for site-selective reactions are well established for solution chemistry, for instance through introduction of electron donating or withdrawing directing groups, it is not a priori clear whether they can easily be transferred to reactions taking place on a metal surface. Here we exploit a combined STM/AFM technique to demonstrate the on-surface formation of complex molecular architectures built up from a heteroaromatic precursor, the tetracyclic pyrazino[2,3-f][4,7]phenanthroline molecule. Selective intermolecular aryl-aryl coupling via dehydrogenative C-H activation occurs on Au(111) upon thermal annealing under UHV conditions. A full atomistic analysis of the different reaction products based on an unambiguous discrimination between pyrazine and pyridine moieties is presented. Our work not only elucidates that ortho-hydrogen atoms of the pyrazine rings are preferentially activated over their pyridine equivalents, but also sheds new light onto the participation of substrate atoms in metal-organic coordination bonding during covalent C-C bond formation.

O 68.14 Wed 18:15 Poster A

"Nunchakus"molecules at metallic surfaces investigated by scanning tunneling microscopy — •lacheng liu[1,2], hongying gao[1,2], philipp held[3], armido studer[3], and harald fuchs[1,2] — [1]Center for Nanotechnology, Heisenbergstr. 11, 48149 Muenster, Germany — [2]Physikalisches Institut, Westfalische Wilhelms-Universitat, Wilhelm-Klemm-Str. 10, 48149 Muenster, Germany — [3]Organisch-Chemisches Institut and Center for Mutiscale Theory and Simulation, Westfalische Wilhelms-Universitat, Corrensstr. 40, 48149 Muenster, Germany

Scanning tunneling microscopy(STM) is demonstrated to be a useful tool to investigate the molecular conformation on metallic surfaces with atomic-scale resolution. In this work we study the adsorption conformations and self-assembly structures of four different "Nunchakus" shaped molecules: Bis(2-naphthyl) peroxide, 2-Naphthoic anhydride, Bis(2-naphthyl)ethanedione and trans-1,2-Bis-(2-naphthyl)ethene. Different metal substrates Au(111), Ag(111) and Cu(111) were tested, to reveal the interaction between organic molecules and metal surfaces. For these nuchakus shaped molecules, different adsorption conformations even on the same metallic surface were identified. The center to center distances of 2-Naphthyl groups of one molecule were measured, which are shorter than the ones in gas phase due to the specific interaction between O atoms and metallic surface atoms which leads to the tortuosity of the molecules.

O 69: Nanostructures at Surfaces: Dots, Particles, Clusters

Time: Wednesday 18:15–20:30 Location: Poster A

O 69.1 Wed 18:15 Poster A

Plasmon-Enhanced Photoemission from Individual Silver Nanoparticles — •Kevin Oldenburg, Hannes Hartmann, Karl-Heinz Meiwes-Broer, Ingo Barke, and Sylvia Speller — University of Rostock, Institute of Physics, 18059 Rostock, Germany

The plasmonic response of metal nanostructures not only depends on material and shape but also on coupling phenomena to the environment. By optical excitation close to the resonance wavelength efficient electron emission can be triggered which is accessible using photoemission electron microscopy (PEEM)[1]. Here we study photoemission from individual silver particles produced in the gas phase and soft-landed onto silicon substrates. The electron emission is correlated to geometric properties obtained by atomic force microscopy (AFM) and discussed regarding particle size and cluster-surface interaction.

[1] M. Rohmer et al., Phys. Stat. Sol. B **247**, 1132 (2010).

O 69.2 Wed 18:15 Poster A

Plasmonically enhanced oriented fluorescence emission in metal-insulator-metal cavities — •Fabian Gossler[1], Matthias Stöter[2], Thorsten Schumacher[3], Markus Lippitz[3], Josef Breu[2], Andreas Fery[1], and Tobias A.F. König[1] — [1]) Institute of Physical Chemistry and Polymer Physics, Leibniz Institute of Polymer Research (IPF), Hohe Str. 6, 01069 Dresden — [2]Dept. of Inorganic Chemistry 1, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth — [3]Dept. of Experimental Physics 3, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth

For implementation of nanophotonic devices, a short life-time and an enhancement of the spontaneous emission is necessary. We fabricate a gold film coupled anisotropic silver nanocube cavity to systematically study the fluorescence enhancement of an oriented fluorophore. For a rational design, the plasmonic properties of the silver nanocubes are designed to match with the emission spectrum of a selected fluorophore. Silicate bilayers with intercalated fluorophores are used as emitting spacer due to their regular height of 4 nm on large scales and orientation of the dye molecules. Finite-difference time-domain (FDTD) simulations, atomic force microscopy (AFM), dark field spectroscopy, confocal and time-resolved photoluminescence measurements have been used to characterize the tailormade nanocavity. Threefold emission enhancement and significantly shorter life-times are observed inside the nanocavity. Electromagnetic simulations support the results and demonstrate the potential of this cavity enhancement as building block for application in plasmonic lasers and gain-loss metamaterials.

O 69.3 Wed 18:15 Poster A

Growth of MnSb Islands on GaAs Substrates — •Christian Klump[1], Carsten Godde[1], Julian Ritzmann[2], Arne Ludwig[2], Andreas Wieck[2], and Ulrich Köhler[1] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

Stacking multiple layers of quantum dots is an established technique for the fabrication of many optic and optoelectronic devices. Up to now, the stacked layers consisted of semiconductor quantum dots exclusively. However, for future spintronic devices, the integration of semiconductor quantum dots with ferromagnetic materials is essential. For this approach, MnSb is an interesting material with its high Curie temperature of 587 K and its compatibility with semiconductor substrates. The pairing of MnSb islands with InAs QDs is studied. As a first step, MnSb islands were grown on different GaAs substrates by MBE. Structural and magnetic properties have been studied by STM, LEED and MOKE.

O 69.4 Wed 18:15 Poster A

Manipulating the nucleation behavior of MoO_x on Al_2O_3/NiAl(110) — •Rik Mom[1], Marcel J. Rost[1], Joost W.M. Frenken[1,2], and Irene M.N. Groot[3] — [1]Huygens-Kamerlingh Onnes Laboratory, Niels Bohrweg 2, Leiden, The Netherlands — [2]Advanced Research Center for Nanolithography, Science Park 104, Amsterdam, The Netherlands — [3]Gorlaeus Laboratories, Einsteinweg 55, Leiden, The Netherlands

Understanding and manipulation of the nucleation behavior of metals and metal oxides on oxidic substrates is essential for the production of catalysts and nanodevices. Due to the large number of non-equivalent sites typically available on an oxidic substrate [1], prediction of such behavior remains challenging. Here, we studied the nucleation of Mo and MoO_x on Al_2O_3/NiAl(110) using scanning tunneling microscopy. In both cases we find 3D growth, yet there are clear differences in the particle dispersion. The larger diffusion speed of Mo leads to larger particles and nucleation on domain boundaries and step edges, whereas for MoOx the dispersion depends on the preparation method. Manipulation of the MoO_x dispersion is possible through the choice of evaporant (Mo or MoO_x). When Mo is evaporated in a mild 5x10^{-7} mbar O_2 atmosphere, the resulting MoO_x shows wetting of domain boundaries and step edges. In contrast, preparation using MoO$_x$ as evaporant, yields a random distribution of particles. The observed differences are explained by a large diffusion length of Mo before oxidation on the surface.

[1] G. Kresse *et al., Science* 308, 1440 (2005)

O 69.5 Wed 18:15 Poster A

Electrodeposition of nickel oxide nanoparticles on micron-sized CVD grown graphene for non-enzymatic glucose sensors with enhanced sensitivity — ●Masoumeh Sisakhti[1], Eva-Maria Kirchner[2], Thomas Hirsch[2], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik,Universität Regensburg — [2]Institut für Analytische Chemie, Chemo- und Biosensorik,Universität Regensburg

We report an optimized electrochemical approach for the non-enzymatic detection of glucose, based on CVD graphene ($100\times200\mu m^2$ in size), decorated with electrodeposited nickel oxide nanoparticles.
The electrochemical growth of the nanoparticles on the carbon nanomaterial was studied and optimized in detail to provide a composite material with large surface area consisting of homogeneous particle size distribution and small particle diameter ranging from 80 to 250 nm.
We studied the electrocatalytic properties of the devices by cyclic voltammetry (CV) and amperometry. Our results demonstrate that the amperometric sensors present electrocatalytic parameters such as a low detection limit of 25μM and wide linear response range of 25μ M to 6.4 mM, indicating that the device operates well in the desired concentration range.
The sensitivity of the micro-sized non-enzymatic amperometric sensor is sufficient for the production of highly integrated sensor arrays for drug screening in small volumes of body fluids.

O 69.6 Wed 18:15 Poster A

Monitoring the interaction of CO with graphene supported metal nanoparticles by vibrational spectroscopy — ●Heshmat Noei[1], Marcus Creutzburg[1,2], Dirk Franz[1,2], and Andreas Stierle[1,2] — [1]Deutsches Elektronen Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Department of Physic, University Hamburg, D-20355 Hamburg, Germany

Small metal nanoparticles dispersed on porous substrates have gained interest in surface science because of their widespread applications, especially in heterogeneous catalysis. It was shown that nanoparticles form ordered arrays on graphene substrates using the moiré of graphene/Ir(111) as a template. The size of these nanoparticles can be carefully controlled on graphene/Ir(111) by the amount of deposited material. Here we report the first describing vibrational spectroscopic studies on Ir, Pt, Rh and Au metal-covered graphene/Ir(111) substrate using CO as probe and/or reactant to monitor the frequency of C-O binding to the metal nanoparticles. The UHV-IRRAS apparatus allowed us to record high-quality IR data and turned out to be a powerful tool to investigate well-arranged metal/grapehne/Ir(111) system. It is found that CO bound on two sites on metal clusters: (1) on-top terraces atoms at low CO coverage and (2) on top-edge atoms at higher CO coverage. The adsorption energy, thermal stability and shape of metal clusters on graphene/Ir(111) are further investigated with respect to the position and intensity of the C-O stretching bands.

O 69.7 Wed 18:15 Poster A

Reconstructed Cu(100)-c(2x2)N surface for self-organized nanoparticle deposition — ●Kariman Elshimi, Julia Andrews, Torsten Veltum, Hendrik Bettermann, and Mathias Getzlaff — Institut für Angewandte Physik, Universität Düsseldorf, 40225 Düsseldorf

Self-organized nanoparticle deposition can be achieved on a nanopatterned Cu(100) surface. This enhances optical, electronic and magnetic properties of the materials, which are expected to be used in the near future technologies.

The Cu surface is cleaned in situ by repeated cycles of Ar$^+$ sputtering followed by annealing. The Cu(100)-c(2x2)N surface can be prepared by bombarding this surface with N$_2^+$ followed by annealing. With in situ scanning tunneling microscope (STM) and low energy electron diffraction (LEED) we characterize the surface. STM images show different surface morphology for different N$_2^+$ doses. The prepared surface at a small N$_2^+$ dose shows self-assembled square patches with surface structure c(2x2) on a clean Cu(100) surface.

We can produce different kinds of metal nanoparticles with several size-ranges from the gas phase using a continuously working arc cluster ion source or a magnetron aggregation source. The charged nanoparticles can be subsequently mass-to-charge filtered by an electrostatic quadrupole deflector. Therefore, the deposition and the behavior of the size-selected nanoparticles on the Cu(100)-c(2x2)N surface can be studied by STM and LEED.

O 69.8 Wed 18:15 Poster A

High-Temperature CsxC58 Solids — ●Weippert Jürgen[1], Ulas Seyithan[1], Kern Bastian[1], Malik Sharali[2], Amati Matteo[3], Gregoratti Luca[3], Kiskinova Maya[3], Strelnikov Dmitry[1], Böttcher Artur[1], and Kappes Manfred M.[1,2] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [3]ESCA microscopy beamline Elettra - Sincrotrone Trieste, ScPA Area Science Park, 34149 Basovizza-Trieste, Italy

Co-depositing Cs and C58+ on HOPG surface led to a new material, CsxC58. The C58 carbon clusters form a scaffold which gets doped by Cs via diffusion across the empty interstitial sites to form bulk CsxC58. Upon heating most of the material survives to yield a doped high-temperature non-IPR fullerene solid, HT-CsxC58. This solid remains stable up to 1100 K, a temperature at which CsxC60 no longer exists. HT-CsxC58 exhibits considerably depleted Cs content (x<2) relative to the as-prepared CsxC58 bulk. The unique thermal stability results from covalent C-C bonds connecting the carbon cages. The Cs dopants contribute to the stability via weak ionic bonds with -C58-C58- oligomers. The HT-CsxC58 material shows a higher defect density, which we attribute to Cs ions relieving the defecting of cages during heating. The topography of the HT-CsxC58 material is dominated by coexisting areas distinguished by their Cs/C58 ratio. The Cs rich islands become striking surface features after air exposure.

O 69.9 Wed 18:15 Poster A

Fabrication and investigation of near-surface spin centers in high-purity single crystal diamond — ●Nicolas Wöhrl[1], Reinhard Remfort[1], Stefan Borgsdorf[2], Tanmoy Chakraborty[3], Ulrich Köhler[2], Dieter Suter[3], and Volker Buck[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [2]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum, Germany — [3]Experimentelle Physik IIIA, Technische Universität Dortmund, Germany

Photons from ideal single-photon sources exhibit quantum mechanical characteristics and therefore allow applications in novel fields including quantum cryptography and spintronics. However, the biggest challenge for the implementation of this concept is maintaining the coherence of the quantum states for a sufficiently long time. One promising candidate for this task is the nitrogen-vacancy center in diamond. The main aim of this project is the fabrication and investigation of near-surface NV–centers in high-purity single-crystal diamond films. Preparation of these active elements close to the surface with good properties is a task which is not yet sufficiently accomplished, especially when read-out is desired to be by optical as well as electronical means. In this project the influence of diamond properties as well as structure and termination of the diamond surface on the spin centers is investigated. Pure single-crystal diamond films are homoepitaxially grown by microwave plasma assisted chemical vapor deposition and the film quality is characterized by standard methods. NV centers are produced by ion implantation and properties investigated spectroscopically.

O 69.10 Wed 18:15 Poster A

3d metal naoparticles deposited on graphene — ●Torsten Veltum, Wolfram Gilbert, Hendrik Bettermann, and Mathias Getzlaff — Institut für Angewandte Physik, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf

In the past few years graphene gained the attention of scientists due to its unique mechanical and electrical properties. In addition to this, fabrication and deposition of nanoparticles on a substrate is of great interest for studies, e.g. as model catalysts. In this contribution we compare the properties of nanoparticles deposited on graphene with those on a 3d metallic thin film.

A thin cobalt film is epitaxially grown by electron beam evaporation on a W(110) single crystal under ultra-high vacuum conditions. To achieve a structurally ordered monolayer graphene on the ferromagnetic substrate we use chemical vapour deposition with propylene. The structure of this system is characterized in-situ by means of scanning tunnelling microscopy (STM) and low energy electron diffraction (LEED).

The nanoparticles are produced using two different gas aggregation sources, an arc cluster ion source (ACIS) and a magnetron sputter aggregation source (Haberland type), with different size distributions and subsequently mass-selected. After the deposition on the sample under softlanding conditions, the structural analysis of the nanoparticles is carried out by STM.

O 69.11 Wed 18:15 Poster A

Deposition and surface interaction of 3d-metal nanoparticles on W(1 1 0) — •Hendrik Bettermann and Mathias Getzlaff — Institute of Applied Physics, University of Duesseldorf

Supported clusters and nanoparticles are rather interesting objects not only from a fundamental point of view but also for technological applications due to their electronic and magnetic properties which show a strong dependence on their size. Interactions between nanoparticles and substrate during and after deposition are an important influence on particle properties.

Our contribution is focused on nanoparticles of 3d-metal alloys. The sizes range from 3 to 15 nm (1e5 to 1e7 amu). Two nanoparticle sources are attached to our UHV system. An Arc Cluster Ion Source (ACIS) produces nanoparticles of 7 nm height and above. A magnetron sputter source (Haberland-type) gives access to smaller sizes. Particles are mass/charge filtered prior to deposition. Size and structural properties are investigates by scanning tunneling microscopy (STM) under UHV conditions. Deposition on substrates other than tungsten will be given as comparison.

O 69.12 Wed 18:15 Poster A

The copper-dioxolene switch controlled by acceptor doping: DFT+U vs. many-body model approach — •Tomasz Ślusarski[1], Tomasz Kostyrko[1], and Victor Garcia-Suarez[2] — [1]Faculty of Physics, A. Mickiewicz University, Poznań, Poland — [2]Departamento de Fisica, Universidad de Oviedo, Oviedo, Spain

A Cu-dioxolene complex with valence tautomeric properties connected to Au(111) surface with an alkanethiol linker[1] is investigated with the density functional theory within GGA+U approach. We study the effect of doping with ICl2 acceptor molecules on the properties of the adsorbed complex. We use the results of the DFT calculations to compute the parameters of an effective many-body model. The model is subsequently studied with a help of exact diagonalization. We also consider model of the junction where the Cu-dioxolene and the acceptor molecule are the central part in the scattering region. We compute the transmission function of the junction in the equilibrium case for different positions of acceptor molecule.

Our main conclusion is that the charge and spin state of the valence tautomeric switch could be well controlled using the acceptor doping. This finding can be useful in development of memory storage or molecular switches.

Acknowledgements This work has been supported by the National Science Centre under the contracts DEC-2012/05/B/ST3/03208 and DEC-2012/07/B/ST3/03412.

References [1] T. Kostyrko, T. Ślusarski, Appl. Surf. Sci. (2015) http://dx.doi.org/10.1016/j.apsusc.2015.11.049

O 70: Nanostructures at Surfaces: Other Aspects

Time: Wednesday 18:15–20:30 Location: Poster A

O 70.1 Wed 18:15 Poster A

Characterization of lamellar nanostructures with X-ray scattering — •Analia Fernandez Herrero, Victor Soltwisch, Mika Pflüger, Anton Haase, Michael Krumrey, and Frank Scholze — Physikalisch-Technische Bundesanstalt

The interest in the reconstruction of nanostructured surfaces has increased in the last decade. Characterizing structures of a few nm challenges the existing metrology tools. The PTB develops high accuracy scattering and reflectometry methods in a broad energy range, from EUV to hard X-rays, at several beamlines at BESSY II and the MLS. Angle resolved scatterometry is a fast and non-destructive method which enables the study of the scattered light from periodic structures. EUV scattering and grazing incidence angle X-ray scattering (GISAXS) are used to investigate structural parameters as the sidewall angle, line width and height of state-of-the-art electron beam written SiN gratings. EUV scatterometry is very sensitive to the imperfections on the structures and therefore it provides a high sensitivity to details of the line geometry. A Maxwell solver based on the finite element method gives consistent results for the reconstruction of arbitrary shape profiles.

O 70.2 Wed 18:15 Poster A

Self-metalation of phthalocyanine molecules with silver surface atoms on Ag(110) — •Lars Smykalla, Pavel Shukrynau, and Michael Hietschold — Technische Universität Chemnitz, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

A direct reaction of molecules with the atoms from the metal surface on which they adsorb (”self-metalation”) was first reported as an unwanted process but later on it was also perceived to be a new method for bottom-up synthesis of metal complexes. We report that metal-free phthalocyanine (H2Pc) molecules are able to incorporate Ag atoms from an Ag(110) surface, therefore forming silver phthalocyanine (AgPc).[1] Scanning tunneling microscopy, X-ray photoelectron spectroscopy, and Density functional theory simulations of this reaction are presented. Three different kinds of molecules were found on the surface that are assigned to H2Pc, the corresponding dehydrogenated molecules (Pc), and AgPc. The relative amounts of Pc and AgPc increase with increasing annealing temperature. Simulations of the reaction path indicate that the metalation of H2Pc is endothermic and that the metalation of the dehydrogenated Pc molecule has a significantly lower barrier and is thermodynamically favorable. Our results shows that the orientation of the substrate surface can be crucial for self-metalation reactions because it was not observed for H2Pc on Ag(111).

[1] Lars Smykalla, Pavel Shukrynau, Dietrich R. T. Zahn, and Michael Hietschold J. Phys. Chem. C, 2015, 119 (30), 17228-17234

O 70.3 Wed 18:15 Poster A

Charge detection of quantum dots in indium arsenide nanowires — •Felix Jekat[1], Kilian Flöhr[1], Sebastian Heedt[2], Marcus Liebmann[1], Stefan Trellenkamp[3], Torsten Rieger[2], Jürgen Schubert[2], Werner Prost[4], Thomas Schäpers[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen — [2]PGI-9, Forschungszentrum Jülich, Germany — [3]PGI-8, Forschungszentrum Jülich, Germany — [4]Center for Semiconductor Technology and Optoelectronics, University of Duisburg-Essen

InAs nanowires have been shown to be suitable as tips for scanning tunneling microscopy (STM) with similar quality compared to tungsten tips, as demonstrated by Flöhr et al. [1]. We present devices with the goal to enable time-resolved counting of single electrons directly at these InAs nanowire STM tips. Two configurations and preliminary transport measurements are presented. The first device configuration utilizes a Quantum Point Contact as charge detector, adapted from Shorubalko et al. [2]. The second device is realized by measuring the conductance variation of another nanowire placed in close vicinity to the first one. This nanowire is coupled by a floating gate to the first nanowire over a distance of several micrometers [3].

[1] K. Flöhr et al. ”Scanning tunneling microscopy with InAs nanowire tips”, Appl. Phys. Lett. 101, 243101 (2012) [2] I. Shorubalko et al. ”Self-Aligned Charge Read-Out for InAs Nanowire Quantum Dots”, Nano Lett. 8, 382 (2008) [3] Y. Hu et al. ”A Ge/Si heterostructure nanowire-based double quantum dot with integrated charge sensor”, Nature Nanotechnol. 2, 622 (2007)

O 70.4 Wed 18:15 Poster A

Investigation of 3D micron structures formation on polyimide and their potential for applications — •Lukas Bayer, Pierre Lorenz, Martin Ehrhardt, and Klaus Zimmer — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany

Lasers have a great potential to produce micro/nano structures fabrication in a fast and cost-effective way. But new discovered or already known self-assembly processes remain unused in commercial or scientific fields. The formation and the application of micro-sized cone structures on PI, produced by laser irradiation using a KrF excimer laser (wavelength 248 nm, pulse duration 25 ns) near the ablation threshold is presented. The influence of the laser irradiation parameters on the cone properties and the density of their appearance are studied by evaluation of images after the irradiation sequence and after each laser shot. The properties of the laser-induced 3D conical surface structures, the height and the width, are analysed by optical and scanning electron microscopy (SEM). The chemical modification of the polymer surface is studied too. In conclusion of found results of the influence of the laser processing parameters to the cone pattern formation process different application will be discussed shortly. These are: application for identification in the field of security features fabrication or the process / equipment validation for laser based processes.

O 70.5 Wed 18:15 Poster A

Different tip functionalizations in scanning probe microscopy — •Philipp Scheuerer und Jascha Repp — Universität Regensburg, Fakultät für Physik, Universitätsstraße 31, 93053 Regensburg

Recently AFM measurements with CO functionalized tips gained a lot of interest since such tips allow to resolve the chemical structure of individual molecules adsorbed on surfaces. The origin of this enhanced resolution is Pauli repulsion [1]. Moreover, it was found that the CO can bend sideways due to tip-sample forces which gives rise to additional contrast sharpening [2].

However, this bending can be a drawback as it causes image distortions. CO functionalized tips have been widely applied not only in AFM but also for KPFS measurements. Up to now, only some other small molecules and atoms were tried to functionalize the tip apex. However there is no alternative that reduces drawbacks like bending and gives a resolution comparable to CO functionalized tips.

We functionalized the tip with several different types of individual molecules to find out whether some of them provide interesting imaging properties.

[1] L. Gross, F. Mohn, P. Moll, N.and Liljeroth, and G. Meyer. Science, 325, 1110 (2009).

[2] P. Hapala, G. Kichin, C. Wagner, F. S. Tautz, R. Temirov, and P. Jelínek. Physical Review B, 90, 085421 (2014).

O 70.6 Wed 18:15 Poster A

Quantifying the contrast mechanisms of a scanning electron microscope by an integrated AFM system — •Frank Hitzel[1], Nils Anspach[1], Kerstin Sempf[2], and Peter Gnauck[3] — [1]Semilab Semiconductor Physics Laboratory Co. Ltd., Budapest, Hungary — [2]Fraunhofer Institute for Ceramic Technologies and Systems, Dresden, Germany — [3]Carl Carl Zeiss Microscopy GmbH, Oberkochen, Germany

The Scanning Electron Microscope (SEM) is a powerful tool to obtain information about sample surface properties like morphology, material type, crystal orientation, conductivity and much more. At low acceleration voltages, secondary electrons are influenced by many different effects, and the resulting images represent a mixture of different contrast sources, which often cannot be distinguished by the SEM related methods themselves.

In such cases, the combined SEM/AFM tool from Carl Zeiss and Semilab goes a step further: Due to the different imaging mechanism, the AFM is able to distinguish between real topography, work function, and conductivity and obtains absolute values for each of them. Especially for samples with strong morphology, the combined SEM/AFM is the only tool permitting full electrical characterization of areas, which have to be located by the detection mechanism of the SEM.

We will present examples in which this unique approach has led to a much better understanding of the investigated sample properties. Examples from the fields of ceramics (SiC), organic electronics, Li batteries and semiconductors will be shown.

O 70.7 Wed 18:15 Poster A

Shifting the voltage drop in electron transport through a single molecule — •Sujoy Karan[1,2], David Jacob[3], Michael Karolak[4], Christian Hamann[1], Yongfeng Wang[1], Alexander Weismann[1], Alexander I. Lichtenstein[5], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93053 Regensburg, Germany — [3]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [5]I. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany

A Mn-porphyrin was contacted on Au(111) in a low-temperature scanning tunneling microscope (STM). Differential conductance spectra show a zero-bias resonance that is due to an underscreened Kondo effect according to many-body calculations. When the Mn center is contacted by the STM tip, the spectrum appears to invert along the voltage axis. A drastic change in the electrostatic potential of the molecule involving a small geometric relaxation is found to cause this observation.

O 70.8 Wed 18:15 Poster A

Controlling and monitoring the local charge distribution of a nanoscaled space charge region — •Katharina Kaiser, Philipp Kloth, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Using a low temperature Scanning Tunneling Microscope in combination with optical excitation we have investigated the interplay and dynamics of free and bound charge carriers inside a nanoscaled space charge region (SCR) at the GaAs(110) surface [1]. This approach allows us to actively modify the local charge distribution at the surface by changing the optical excitation density and the tunnel current and to control charge fluctuations.

One central part is the capture process of photo-generated minority charge carriers in the presence of locally fixed dopant atoms within the space charge region. By establishing a quantitative model, we are able to extract key quantities like the diffusive or field driven capture rate of photo-generated holes. The analysis of the noise of the tunnel current provides access to the temporal charging and discharging process of dopant atoms inside the SCR, showing that the presence of photo-generated charge carriers changes the noise of the system significantly.

[1] Kloth et al., Nat. Comm. (2015)

O 71: Scanning Probe Techniques and New Experimental Methods

Time: Wednesday 18:15–20:30 Location: Poster A

O 71.1 Wed 18:15 Poster A

A 30mK dilution fridge UHV SP-STM (9/4T) housed in the new SPIN Laboratory — •Andreas Eich[1], Henning von Allwörden[1], Jan Hermenau[2], Andreas Sonntag[2], Jan Gerritsen[1], Daniel Wegner[1], and Alexander Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Institute of Nanostructure and Solid State Physics, Hamburg University, Hamburg, Germany

Unraveling many of the current dilemmas in nanoscience hinges on the advancement of techniques which can probe the spin degrees of freedom with high spatial, energy, and ultimately high temporal resolution. With the development of sub-Kelvin high-magnetic field STM, two complementary methods, spin-polarized scanning tunneling spectroscopy (SP-STS) and inelastic STS (ISTS), can address single spins at the atomic scale with unprecedented precession.

Common cryostat designs for spin-polarized STM sub-Kelvin application are based on 3He liquification, which are limited in base temperature, hold time, and cooling power. To address these limitations, we demonstrate a newly designed 30mK dilution fridge based UHV spin-polarized microscope in a vector magnetic field, capable of atomic spin detection and atomic manipulation. Our design consists of tip/sample exchange at cold temperatures as well as cold material deposition and features extremely low 4He consumption with a long hold time. To prevent any external perturbation of the measurements, the system is housed in the new ultra-quiet SPIN laboratory (IMM-RU) featuring a 150 ton damped foundation and proper acoustical and RF shielding.

O 71.2 Wed 18:15 Poster A

Design of a low-temperature scanning tunneling micro-

scope with photon collection system — •Moritz Winkler[1], Lukas Gerhard[1], Kevin Edelmann[2], and Wulf Wulfhekel[2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT) — [2]Physikalisches Institut, Karlsruhe Institute of Technology (KIT)

We provide a new design for a low-temperature ultra-high vacuum scanning tunneling microscope (STM) with a photon collection unit that guides the collected light into a spectrometer. The design has the potential of achieving a high photon yield by using a 3D-printed miniature parabolic mirror that collects photons from a large solid angle close to the tunnel junction. The photon yield is further increased by limiting the optical path to a single optical fiber. The STM will be equipped with an absolute position determination system of the tip in order to approach and examine structures manufactured by lithographic processes. By Joule-Thomson expansion of helium, the STM will operate at a temperature of around 1 K [1].

[1] A compact sub-Kelvin ultrahigh vacuum scanning tunneling microscope with high energy resolution and high stability L. Zhang, T. Miyamachi, T. Tomanić, R. Dehm and W. Wulfhekel

O 71.3 Wed 18:15 Poster A

Validation and automatization of controlled molecular manipulation techniques on an STM — •Aizhan Sabitova[1,2,3], Philipp Leinen[1,2], Matthew F.B. Green[1,2], Taner Esat[1,2], F. Stefan Tautz[1,2], Christian Wagner[1,2], and Ruslan Temirov[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]National Laboratory Astana, Kazakhstan

The success of scanning probe microscopy (SPM) based hand-controlled single molecule manipulation technique [1,2] relies upon three main components. These are high-precision positioning of the SPM tip, a hand motion tracking system [1], and virtual reality goggles displaying the motion trajectory and feedback signals in real time [2]. With this, reproducible extraction of molecules from a closed monolayer on a metal surface and statistical determination of successful trajectories was achieved. Until now these experiments were performed on a low-temperature non-contact atomic force/scanning tunneling microscope (LT NC-AFM/STM), that has tunneling current as well as the frequency shift of the tuning fork sensor as feedback signals. Here, we study how successful trajectories can be transferred to an instrument without AFM capability (LT STM) and automatized to enable fast and efficient manipulation within monolayers.

[1] M.F.B. Green *et al.*, Beilstein J. Nanotechnol. 2014, **5**, 1926-1932

[2] P. Leinen *et al.*, Beilstein J. Nanotechnol. 2015, **6**, 2148-2153

O 71.4 Wed 18:15 Poster A

Fast electronic pump-probe spectroscopy using shaped sub-nanosecond pulses — •Gregory McMurtrie[1,2], Jacob Burgess[1,2], Steffen Rolf-Pissarczyk[1,2], and Sebastian Loth[1,2] — [1]Max-Planck Institut für Struktur und Dynamik der Materie — [2]Max-Planck Institut für Festkörperforschung

Pump-probe schemes make it possible to measure fast dynamical processes with the scanning tunneling microscope (STM). Electronic pump-probe spectroscopy excites and detects dynamics using voltage pulses [1] with the time scale being set by the speed at which the voltage can be changed at the tunnel junction [2], [3].

We use time domain reflectometry to measure the transmission characteristics of a low-temperature STM. Damping in the cabling and standing waves at various points of the transmission line smear the edges of the pump and probe pulses and limit the achievable time resolution. By extracting amplitude and phase information from the reflectometry measurements it is possible to compensate these imperfections and create a shaped input pulse which will have sharp edges at the STM tunnel junction. This process can shape pulses with a bandwidth of up to 3 GHz, enabling sub-nanosecond time resolution.

Pushing electronic pump-probe spectroscopy beyond the nanosecond range will enable a wide range of experiments that harness the strong interaction of electrons with spin, charge and vibration excitations.

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

[2] C. Saunus, et al., Appl. Phys. Lett. 102 051601 (2013).

[3] C. Grosse, et al. Appl. Phys. Lett. 103 183108 (2013).

O 71.5 Wed 18:15 Poster A

Combining Scanning Tunneling Microscopy and pulsed optical excitation — •Judith von der Haar, Philipp Kloth, Terence Thias, Ole Bunjes, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The combination of Scanning Tunneling Microscopy (STM) and optical excitation merges two of the most successful experimental techniques in solid-state physics. Especially pump-probe excitation gives the prospect to resolve surface dynamics on the atomic scale. A serious challenge of optical excitation in STM is controlling the thermal load at the tunnel junction. We present a very compact and versatile laser setup that addresses various requirements of this experimental technique. First of all, the laser source must provide a very low-noise and stable output power. Next, in order to find the spot of maximum excitation in a standardized manner, it is important to implement a submicrometer precise stage that allows the scanning of the focus point of the laser beam along the tip-surface junction - even during tunnel conditions. At last, standard pump-probe pulses must be transformed into complex laser pulse patterns [1]. Using an optical modulator with a bandwidth in the gigahertz range and a high frequency function generator, we process the continuous wave laser beam into nanosecond pulses. [1] Terada et al., Nature Photonics, 4(12), 2010.

O 71.6 Wed 18:15 Poster A

New Directions in Tip-Enhanced Near-Field Optical Microscopy — •Julia Janik, Nina Mauser, and Achim Hartschuh — Department Chemie and CeNS, LMU München, Germany

The characterization of nanostructures with high spatial resolution and detection sensitivity can be achieved by tip-enhanced near-field optical microscopy (TENOM) [1].

We report on our efforts to extend this method into further directions. One direction is the application of tip-enhancement to photovoltaic and light-emitting devices as suggested in [2]. We obtained the first high-resolution photocurrent images of carbon nanotube devices using a metal tip to locally enhance optical-to-electrical transduction [3]. We show that the efficiency of the reversed process leading to electroluminescence can be increased as well.

Furthermore we are focusing on the implementation of tip-enhanced near-field optical microscopy at low temperatures (5 K). Therefore we present a new microscope design based on a solid immersion lens configuration providing very high collection angles and efficiencies. We acknowledge financial support by DFG, NIM and the ERC (NewNanoSpec).

[1] N. Mauser, A. Hartschuh, Tip-enhanced near-field optical microscopy, Chem. Soc. Rev. 43, 1248 (2014).

[2] P. Bharadwaj, B. Deutsch, L. Novotny, Optical Antennas, Adv. Opt. Photon. 1, 438 (2009).

[3] N. Mauser et al., Antenna-Enhanced Optoelectronic Probing of Carbon Nanotubes, Nano. Lett. 14, 3773 (2014).

O 71.7 Wed 18:15 Poster A

AFM for TERS: Development of probe heads for Tip-Enhanced-Raman-Spectroscopy — •Jalmar Tschakert[1], Thomas Göddenhenrich[1], André Schirmeisen[1], Marcel Weinhold[2], Thomas Sander[2], and Peter J. Klar[2] — [1]Institut für Angewandte Physik, Justus-Liebig-Universtiät Gießen — [2]I. Physikalisches Institut, Justus-Liebig-Universität Gießen

Tip-Enhanced-Raman-Spectroscopy (TERS) has become a powerful tool in material science to combine topographic and chemical imaging. Our experimental TERS setup is based on an inverted optical microscope with an x,y scan stage for scanning transparent samples. Two different type of AFM heads are developed: one with a cantilever and a fiber-optical interferometer and the other based on a quartz-tuning-fork. Both designs are compact and give a good long time thermal and mechanical stability without the need of an additional damping mechanism. Contact and non-contact measurements are controlled via GXSM software with a Soft-dB-Mk3-DSP board leading to a flexible scan control with different AFM probes as well as the option to add own user specific tasks.

O 71.8 Wed 18:15 Poster A

Hexaboride preparation techniques for Scanning Tunneling Microscopy studies — •Philipp Buchsteiner[1], Geetha Balakrishnan[2], David P. Young[3], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Department of Physics, University of Warwick, United Kingdom — [3]Department of Physics and Astronomy, Louisiana State University, USA

Hexaborides (LaB6, etc.) are widely for technical applications, e.g. Electron Microscopy. Although the surface properties for these applications are important, few Scanning Tunneling Microscopy (STM) studies had been carried out [1,2]. Investigating surfaces with atomic resolution requires sample preparation ensuring atomically flat areas. Therefore different techniques have been developed for two types of single crystals. Samples of about 3mm length were glued onto GaAs. Here the hexaboride (100)-plane is orientated parallel to the GaAs(110) planes. After cleavage, Atomic Force Microscopy (AFM) studies showed large flat terraces with step heights ranging from a single bulk lattice constant of 0.4nm up to some monolayers. Low-energy Electron Diffraction (LEED) confirmed a non-reconstructed 1x1 surface periodicity. Larger samples with a few cm length and some mm in diameter were cut along the (100)-planes using a diamond wire saw to rectangular pieces. Here no GaAs carrier was obligatory and also large flat surface areas were verified with AFM.

[1] J.S. Ozcomert, M. Trenary, Surf. Sci., 265 (1992), [2] Yee, M. M. et al. arXiv.org, 1308.1085v1 (2013)

O 71.9 Wed 18:15 Poster A

Solution AFM Studies of Molecule Crystals: Exploiting Photon Pressure — •Sven Kraft, Heinrich Behle, Kai Wardelmann, Mohammadreza Bahrami, Björn Vogler, Mirjam Samelin, Semjon Köhnke, Boris Hage, Ingo Barke, and Sylvia Speller — University of Rostock, Institute of Physics, 18059 Rostock, Germany

Atomic Force Microscopy in liquids is an important tool for imaging processes in molecular layers and films. Dynamic AFM usually suffers from distorted resonance curves of the cantilever oscillation in the medium. Driving the cantilever via photon pressure is an option to improve the cantilever oscillation and acquire topographies in solutions in dynamic mode. We aim to test this approach with the aggregation and dissolution of molecule crystals in a number of solvents, in order to gain insight into the internal structure of such crystals.

[1] G.C. Ratcliff, D.A. Erie, R. Superfine, Appl. Phys. Lett. **72**, 1911 (1998)

[2] D. Ramos, J. Tamayo, J. Mertens, and M. Calleja, J. Appl. Phys. **99**, 124904 (2006)

O 71.10 Wed 18:15 Poster A

A Superconducting Tunneling Junction (STJ) Detector for Soft X-Ray Absorption Spectroscopy at 50mK — •Ivan Baev[1], Jan-Hendrik Rüscher[1], Jens Viefhaus[2], Michael Martins[1], and Wilfried Wurth[1,2] — [1]Physics Department, University of Hamburg — [2]DESY Photon Science, Hamburg

Soft X-Ray absorption spectroscopy (XAS) is an important technique at synchrotrons nowadays that allows to investigate electronic and magnetic properties in an element specific way. The investigation of non-conductive, soft organic or buried materials can't be carried out in total electron yield. In these cases an efficient fluorescence detector is needed to perform XAS measurements in partial fluorescence yield (PFY). The STJ detector is capable of count rates as high as 10 kcps per 100 μm^2 pixel size with an energy resolution of approximately 50eV for 1.5 keV photons. The STJ is furthermore integrated into a 50mK cryostat for XAS measurements at the P04 beamline at Petra III, DESY. We will present first measurements on a model system.

O 71.11 Wed 18:15 Poster A

Construction of a movable UHV chamber for in situ sample preparation of molecules on TiO2 — •Steffen Bornemann, Bernhard Spicher, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

TiO2 is an important material for chemical catalysis which e.g. can be applied in photocatalytic water splitting [1]. In order to investigate this system with different surface sensitive techniques, we have constructed a movable UHV chamber for in situ sample preparation of molecules on the TiO2(110) rutile surface. Samples can be transferred to different low temperature scanning tunneling microscopes as well as to an analysis chamber equipped with a low energy electron diffraction (LEED) and an Auger electron spectroscopy (AES) setup. TiO2 substrates can be prepared by direct current heating, by electron beam heating and by ion beam sputtering. The chamber is equipped with an external evaporator for molecule deposition from a liquid phase like methanol and with an electrospray deposition system for more complex, non-volatile molecules. Moreover, sub-monolayer of metals can be deposited from different electron-beam evaporators. After several cycles of sputtering and heating up to 600°C we could verify the 1x1 reconstruction of the clean TiO2(110) surface after in situ transferring the samples to the LEED setup [2]. Ex situ characterization by atomic force microscopy shows terraces connected by single and multiple atomic steps.

[1] M. Ni, M.K.H. Leung, D. Y.C. Leung, K. Sumathy, Renewable and Sustainable Energy Reviews 11, 401 (2007) [2] Hiroshi Onishi, Yasuhiro Iwasawa, Surface Science Letters 313, 783 (1994)

O 71.12 Wed 18:15 Poster A

Following ultra thin film growth by in-situ High Energy X-ray Diffraction — •Florian Bertram, Olof Gutowski, and Uta Ruett — DESY Photon Science, Notkestrasse 85, 22607 Hamburg, Germany

High energy x-ray diffraction (≈ 80 keV) is a versatile tool to record diffraction patterns from surfaces, interfaces, and ultra-thin films at remarkable high speed compared to conventional diffraction measurements (≈ 15 keV). Due to the high photon energy diffraction angles become smaller, which results in a much flatter Ewald's sphere in a given q-range. Therefore, crystal truncation rods (CTR's) can be recorded in grazing incident geometry by a simple rotation of a few degree with a 2D detector at a fixed position.

We demonstrate how this method can be used to record real time diffraction data during MBE growth of ultra-thin films. Here, the growth of magnetite (Fe_3O_4) on MgO(001) was studied. We could follow the evolution of the CTR's during growth with a time-resolution of 5 sec.

O 71.13 Wed 18:15 Poster A

Reprocessing with radial shock waves — Philipp Weil, •Robert Ossig, Hans-Günter Hloch, and Jürgen Bohnen — wfk - Cleaning Technology Institute, D-47807 Krefeld, Deutschland

We present a novel application to utilise radial shock waves as an effective, sustainable, hygienic and gentle method to clean sensitive surfaces (e.g. textiles). Usually, shock waves are used for medical applications, e.g. to break up kidney stones or to promote bone healing after complicated fractures. Radial shock waves are generated using the ballistic principle, where a small projectile is fired at high speed upon a metal applicator, from which radial shock waves expand into an homogenous medium (usually water). Directly behind the wave front peak pressures of up to 100 MPa and, thus, high energy input per area is achieved. While impinging on a surface, a part of the shock wave is reflected back into the water and interacts with the next impinging wave. This leads to high mechanical interactions directly at the surface, which explain the efficient destruction of kidney stones in soft tissue. In this contribution we discuss relevant interactions between shock waves, textiles and soils and present shock wave parameters (e.g. frequency, distance to surface) for optimum soil removal and minimum surface damage. Furthermore, a comparison of the new method with typical methods, which are in use today, are presented.

O 71.14 Wed 18:15 Poster A

Laser desorption of chiral molecules — •Farinaz Mortaheb, Joern Lepelmeier, Kerstin Wachinger, Aras Kartouzian, Ulrich Boesl, and Ulrich Heiz — Chair of Physical Chemistry, Lichtenbergstraße 4, 85748 Garching

Laser desorption enables the vaporization of non-volatile and thermally unstable molecules without fragmentation and thus allows to analyze large bio- and organic molecules in the gas phase. Desorbed molecules can be analyzed mass spectroscopically by REMPI-ToF, which can be combined readily with circular dichroism to investigate the chiroptical properties of non-volatile chiral molecules in the gas phase without any interference from solvent molecules (as in solutions) or diastereomeric partner molecules. Using the example of Binol, and a prototype experimental apparatus, an optimized sample preparation recipe was found to optimize the laser desorption yield of neutral molecules. The high signal intensity and stability attained in our lab pave the way for further experiments using a purpose designed setup.

O 71.15 Wed 18:15 Poster A

Identification of nanoscale phases using Low Energy Electron Microscopy. — •Martin Hoppe, Jan Höcker, Jens Falta, and Jan Ingo Flege — Universität Bremen, Germany

Low Energy Electron Microscopy (LEEM) is an established method to investigate surface structures and morphologies with a lateral resolution in the few nanometer range. The main benefits are the *in situ* capabilities of the instrument enabling surface monitoring during manipulation such as growth and chemical reactions. In LEEM, crystal phases differing in structure or chemical composition may exhibit different intensities at a given energy. But, this does not allow for a definite identification especially on very heterogeneous surfaces. The latter can be achieved using intensity-voltage (I(V)) curves as a

reliable fingerprint for each phase.[1] We show that the correlation coefficient or R_2-factor[2] can be used to compare unknown LEEM-I(V) curves to reference spectra and thus to distinguish phases on the 10 nm scale. Performing a pixel-wise automated comparison, 2D maps of the surface phases can be generated and, in a dynamic I(V)-LEEM experiment, their development during sample manipulation can be monitored. This new method will be demonstrated using examples from ruthenium oxidation[3] and chemical reactions at cerium oxide surfaces[4].
[1] *J. I. Flege et al.*, Phys. Status Solidi RRL **6**, 463 (2014)
[2] *M.A. Van Hove, W. H. Weinberg, and C.-M. Chan*, Low-Energy Electron Diffraction, Springer (1986)
[3] *J. I. Flege et al.*, ACS Nano **9**, 8468-8473 (2015)
[4] *J. Höcker et al.*, Adv. Mater. Interfaces, in press (2015)

O 71.16 Wed 18:15 Poster A

Reliability of LEED analyses for complex systems — •Lutz Hammer, Pascal Ferstl, and M.Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg

The correspondence of experimental and calculated best-fit intensity spectra of a LEED structure analysis is quantitatively expressed by means of reliability factors. Most frequently the Pendry R-factor R_P is applied nowadays. Best-fit values in the range $R_P = 0.2$ - 0.3 or even somewhat larger are generally accepted as a proof for the correctness of the underlying structural model. In the present contribution it is shown that this only holds for structurally quite simple systems. For more complex structures, in contrast, the distinction between similar models which only vary by the presence (or absence) of very few atoms within the (large) unit cell requires a significantly better level of spectral correspondence ($R_P \ll 0.2$).

In the case study presented here different structural variations of the surface reconstruction of $Fe_3O_4(100)$ are investigated, whereby the key features of the reconstruction model (subsurface iron vacancies and interstitials) are systematically either neglected or varied in position. It is shown that those crystallographically wrong structures still produce R-factors in the range $R_P = 0.2$ - 0.3, occasionally even lower. The reason for this structural insensitivity lies qualitatively in the relatively small scattering contribution of a particular atom to the total wave field produced by a large surface unit cell. Approaches to improve the quality of a LEED intensity analysis as well as consistency checks to detect incomplete structural models are presented and discussed.

O 71.17 Wed 18:15 Poster A

Source Development for Ultrafast Transmission Electron Microscopy — •Nora Bach, Armin Feist, Reiner Bormann, Sascha Schäfer, and Claus Ropers — IV. Physical Institute, University of Göttingen, Göttingen

Ultrafast transmission electron microscopy (UTEM) is a novel experimental technique that combines a nanoscale spatial with femtosecond temporal resolution [1]. The imaging and diffraction resolution in this technique is governed by the brightness of the laser-driven electron source used [2].

Here, we present the design and implementation of an advanced UTEM instrument based on the modification of a commercial Schottky Field emission TEM [3]. Single-photon photoemission from a tip-shaped ZrO/W(100) emitter is employed, yielding a spectral bandwidth of 0.6 eV, a low intrinsic emittance of about 5 nm·mrad, and an electron probe size down to 1.5 nm.

We characterize the temporal structure of the electron pulses by electron-photon cross-correlation and obtain a pulse width of 300 fs (full-width-at-half-maximum). The demonstrated high beam quality of the source will enable new applications in the study of nanoscale ultrafast dynamics, including ultrafast electron holography and phase-contrast imaging.

[1] A. H. Zewail, Science 328, 187 (2010).
[2] M. Gulde et al., Science 345, 200 (2014).
[3] A. Feist et al., Nature 521, 200 (2015).

O 71.18 Wed 18:15 Poster A

VUV photon detection with acetone counters for inverse photoemission — •Christian Thiede, Iris Niehues, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Universität Münster

Inverse photoemission experiments in the isochromat mode require the use of band-pass photon detectors. The bandpass behavior is usually realized by combining the photoionization threshold of a suitable counting gas (high pass) with the transmission characteristics of an alkaline earth fluoride window (low pass). Since inverse photoemission intrinsically suffers from a low photon yield, an optimized detector efficiency is crucial for this technique. In particular, the bandpass width and the efficiency depend on the transmission characteristics of the entrance window [1], the detection gas type and pressure, the readout electronics and the counter geometry. We studied these parameters for the well-known combination of CaF_2/acetone. We provide a recipe how to operate the detector in proportional as well as in Geiger-Müller mode. [1] Thiede *et al.*, Rev. Sci. Instrum. **86**, 085101 (2015)

O 71.19 Wed 18:15 Poster A

MOKE UHV-Setup — •Vivienne Bippus, Christian Klump, Sani Noor, Christian Urban, and Ulrich Köhler — Experimentalphysik IV, Arbeitsgruppe Oberflächenphysik, Ruhr-Universität Bochum, Germany

We present a UHV-setup for measuring the magneto-optic Kerr-effect (MOKE) at variable temperatures. The setup is integrated with a number of metal and semiconductor MBE-sources pointing at the sample in the MOKE position. Therefore, in situ MOKE measurements can be carried out simultaneously during the growth process of the sample. The data acquisition software is able to record the temporal evolution of magnetic hysteresis curves. A cryostat fitted with the sample holder offers substrate temperatures down to 4.2 K. Hence, temperature, layer thickness and crystal orientation dependent measurements with a resolution of a mono-layer are possible. The poster will present details on the structure and the control of the different components used, together with examples of the coverage dependent magnetic behaviour of ferromagnetic layers on semiconductors.

O 72: Solid-Liquid Interfaces: Reactions and Electrochemistry

Time: Wednesday 18:15–20:30 Location: Poster A

O 72.1 Wed 18:15 Poster A

Measurement of surface diffusion at solid-liquid interfaces using in situ linear optical diffraction — •Lasse Kattwinkel, Christoph Lemke, and Olaf Magnussen — Insitut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

Surface diffusion at solids in liquid environment is a fundamental process in many interface reactions, but much less understood than surface diffusion under vacuum conditions. We develop a novel method to measure the surface diffusion rates in such systems using optical diffraction. In this method a density grating in an adsorbate layer is created by thermal desorption induced by the two interfering beams of a nanosecond Nd:YAG laser. The evolution of the grating is then probed by linear optical diffraction of a HeNe laser beam at the grating. From the exponential decrease of the diffraction intensity the surface diffusion coefficient can be extracted. We describe the setup for this novel in situ technique and first experimental results.

O 72.2 Wed 18:15 Poster A

Laterally varying electrochemical deposition of solid copper on magnetically patterned exchange bias templates — •Iris Koch[1], Florian Ahrend[1], Timo Ueltzhöffer[1], Svetlana Ivanovna Shevtsova[2], Philipp Martin Reintanz[1], Ulrich Siemeling[1], and Arno Ehresmann[1] — [1]Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel — [2]Research Institute of Physics, Southern Federal University, Stachki Ave. 194, RUS-344090 Rostov-on-Don

The inhomogeneous magnetic field landscape above magnetically patterned exchange bias (EB) systems [1] was utilized to influence the electrochemical reaction between a copper sulfate solution and a tantalum layer in a laterally anisotropic way. Thus, a local change of the copper deposition rate due to the specially designed magnetic stray fields acting on the paramagnetic Cu^{2+} ions is initiated. For process optimization, parameters like ion concentration, deposition time, and tantalum layer thickness were varied and analyzed by optical microscopy and energy dispersive x-ray spectroscopy. In all of the performed experiments, a significant influence of the EB system's magnetic pattern and, therefore, surface properties on the electrochemical reaction could be observed. This novel concept appears to be a promising method for the controlled growth of metallic nanowires.

[1] F. Ahrend et al., J. Magn. Magn. Mater. 381, 292 (2015)

O 72.3 Wed 18:15 Poster A

Achieving selective electrocatalytic activity for CO2 reduction using highly porous Cu black catalysts — •Abhijit Dutta, Motiar Rahaman, Miklos Mohos, Nicola Christian Ludi, and Peter Broekmann — Department of Chemistry and Biochemistry, University of Bern Freiestrasse 3 CH 3012 Bern Switzerland

The selective electroreduction of carbon dioxide to ethane and carbon monoxide on porous Cu-black catalysts has been investigated at various electrochemical potentials in aqueous 0.5 M NaHCO3 solution. The evolution of hydrogen gas at an electrode surface plays a significant role to form this novel porous architecture during the electrodeposition of copper, particularly when a high current density is maintained. The hydrogen gas evolution inhibits electrodeposition of copper directly onto the cathode by temporarily preventing contact between the copper cathode and the electrolyte. Ultimately, a thin film of electrolyte surrounding hydrogen bubble comes into contact with the cathode, which completes the EC circuit and permits for electrodeposition of copper black. This porous morphology remains alike even after 1 h electrolysis at -1.0 V vs RHE. The Cu black catalyst exhibited the best selectivity for CO and ethane at -0.50V and -0.70V vs RHE with faradaic efficiencies of 40% and 37% respectively. Furthermore, the total FE of these two products is almost 75 to 80% at moderately cathodic potential range. Understanding the structural morphology of Cu black and the selectivity of products distribution could be valuable for the further development of advanced electro-catalytic materials for carbon di-oxide reduction.

O 72.4 Wed 18:15 Poster A

Sustainable sarcosine inhibitors for corrosion reduction on DC01 steel — •Saad Kaskah[1], Paulo Ferreira[2], Gitta Ehrenhaft[2], Jörg Gollnick[2], and Christian B. Fischer[1] — [1]Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany — [2]Institute of mechanics and material science, TH Mittelhessen University of Applied Sciences, 35390 Giessen, Germany

Sustainable corrosion inhibitors are considered for good efficiencies without any environmental limitations in steel protection. In this work four N-acyl sarcosine derivatives are investigated via direct surface adsorption on cold rolled steel DC01 as potential corrosion inhibitors. Potentiodynamic polarization measurements were conducted in an aqueous solution buffered with potassium phosphate. Furthermore, for a realistic test a spray corrosion chamber with fresh water was used in long term. The short-term electrochemical tests were performed for one hour and the spray corrosion chamber for 24 hours. For the chamber test, each metallic sample was digitalized with a scanner at specific times and the corrosion process evaluated by corroded area. The results showed an improved corrosion reduction for the tested inhibitors on DC01 steel. Their efficiencies show a direct correlation according to their molecular weight. The worst inhibitor is the natural mixture of coconut derived sarcosines with 20 % efficiency. The best one with the highest molecular weight and longest carbon chain is Oleylsarcosine with 96 % efficiency.

O 72.5 Wed 18:15 Poster A

In situ Surface X-ray Diffraction Study of Ultrathin Epitaxial Co Films on Au(111)/H-Si(111) in Transmission Geometry — •Jonathan Laufer[1], Finn Reikowski[1], Tim Wiegman[1], Fouad Maroun[2], Philippe Allongue[2], Jakub Drnec[3], Jochim Stettner[1], and Olaf M. Magnussen[1] — [1]IEAP, CAU Kiel, Germany — [2]Ecole Polytechnique, CNRS, Palaiseau, France — [3]ESRF, Grenoble, France

Gracing incidence diffraction in reflection geometry belongs to the standard repertoire for the in situ characterization of single crystal surfaces and adsorbate structures. Although being commonly used for measurements of crystal truncation rods, mapping in-plane structures proves to be tedious with this method. Here we present surface diffraction studies in transmission geometry, in which a large portion of the in-plane structure can be seen on a single detector frame. To flatten the curvature of the Ewald sphere, high energies in the range 25 keV to 70 keV were used. This means that the out-of-plane wavevector transfer changes only slightly over the range of reciprocal space covered by the detector. Furthermore, the high energies result in low absorption which is necessary since the beam has to travel through the entire sample in this configuration. Using this novel approach, we investigated samples consisting of 30 monolayers Au(111) deposited on H-Si(111) with a thickness of 600 μm. 10 - 20 monolayers of Co were electrochemically deposited on these substrates and analyzed by surface sensitive in situ transmission X-ray scattering. With this method the Co deposition and dissolution could be monitored under reaction conditions.

O 72.6 Wed 18:15 Poster A

Trends in catalytic activity of Ni-based electrodes for the hydrogen evolution reaction — •Hannah Schlott[1], Marc Ledendecker[2], Menny Shalom[2], Markus Antonietti[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Max-Planck-Institute of Colloids and Interfaces, Potsdam

Using density-functional theory (DFT) we investigated the hydrogen adsorption on (0001) surface terminations of different Ni-based compounds, which are promising new electrode materials for the hydrogen evolution reaction (HER). While pure Ni is known to be not a good electrode material for the HER since it binds hydrogen too strongly [1,2], electrochemical experiments indicate an improved performance for the binary compounds Ni_3N, Ni_3S_2 and Ni_5P_4. In our DFT calculations we find decreased hydrogen adsorption energies for the Ni compounds, placing them closer to the activity maximum in a volcano plot relation than pure Ni [1,2]. However, experiment and theory suggest a different order of the performance for the investigated compounds. Reasons for this discrepancy will be discussed and consequences of these findings will be presented.

[1] J.K. Nørksov, T. Bligaard, A. Logadottir, J.R. Kitchin, J.G. Chen, S. Pandelov, U. Stimming, J. Electrochem. Soc. **152**, J23 (2005).
[2] P. Quaino, F. Juarez, E. Santos, W. Schmickler, Beilstein J. Nanotechnol. **5**, 846, (2014).

O 72.7 Wed 18:15 Poster A

Cu surface reactions in hydrochloric solution probed on the atomic scale by polarization optical methods and STM — •Christoph Cobet, Gholamreza Barati, Vladyslav Solokha, and Kurt Hingerl — Center for Surface- and Nanoanalytics (ZONA), Johannes Kepler Universität, Altenbergerstr 69, A-4040, Linz, Austria

Electrochemical reactions on metal electrodes have been in the focus of many scientific studies and Cu is probably the most investigated example. The interest on Cu is motivated by questions concerning e.g. corrosion, electro-polishing, and catalytic processes. It is evident that a fundamental understanding requires knowledge about the microscopic occurrence of the surface in electrolyte. But unfortunately, most of the classical surface sensitive techniques as used in UHV cannot be applied in liquid environments and thus many details about surface structures are still under discussion. In the presented work we combine reflection anisotropy spectroscopy and a homemade electrochemical scanning tunneling microscope in order to study Cu(110) single crystals in hydrochloric solutions. With this approach we could monitor the local appearance as well as the dynamics of interface transformations/reactions on atomic scale. In particular it was possible to correlate anodic Faraday-current maxima with structural transformation. Accordingly, the Cl adsorption minimizes the surface energy by a formation of monoatomic steps parallel to the [001] direction which finally ends in a faceting of the surface. These surface modifications may influence also the rate of the known Cu dissolution at increasing anodic potentials.

O 72.8 Wed 18:15 Poster A

Directional Movement of Third Generation Light-Driven Molecular Motors on Surfaces — •Henrieke Heideman[1], Johan Visser[1], Jos Kistemaker[1], Peter Stacko[1], Meike Stöhr[2], and Ben Feringa[1] — [1]Stratingh Institute for Chemistry, Groningen, The Netherlands — [2]Zernike Institute for Advanced Materials, Groningen, The Netherlands

Third generation molecular motors are equipped with two rotor units, which can rotate unidirectionally when powered by light. Although the solution behavior of these molecules has recently been studied, integrating them into useful nanodevices represents a major challenge. One key requirement is that these molecular motors are functional under ambient conditions. Moreover, it is crucial to have the achiral unidirectional rotary motion of these molecular motors happening on surfaces in order to get out of the Brownian regime. In the present study, the behavior of third generation molecular motors on modified HOPG surfaces was studied with STM under ambient conditions.

O 72.9 Wed 18:15 Poster A

Towards understanding the mechanism of water splitting on TiO_2 — •Simon J. Schmitt, Saman Hosseinpour, and Ellen H.G. Backus — Max-Planck-Institute for Polymer Research, Ackermannweg 10, Mainz, Germany

Finding a clean and renewable energy source to replace fossil fuels has attracted much attention, the past few decades, as a requirement for the sustainable development of societies. Direct hydrogen generation on TiO_2 by photocatalytic dissociation of water using sunlight was already proposed more than 40 years ago. However, despite extensive work in this area, the fundamentals of the process remain ill-understood, mainly due to the lack of a proper tool to specifically explore the interface between water and TiO_2. Sum frequency generation spectroscopy (SFG), is an inherently surface sensitive tool, allowing the study of specifically the water molecules at the TiO_2 surface. We present data on water in contact with TiO_2 thin films at various pH values and isotopic dilution and correlate the spectral observations with surface species. Moreover, we show first UV-pump-SFG-probe data, illustrating the first steps towards following the photo-induced dissociation of water at the TiO_2 interface in real-time.

O 72.10 Wed 18:15 Poster A

Experimental Approach for Determining Semiconductor/liquid Junction Energetics by Operando Ambient-Pressure X-ray Photoelectron Spectroscopy — •Matthias H. Richter[1,2,7], Michael F. Lichterman[1,2], Shu Hu[1,2], Ethan J. Crumlin[3], Stephanus Axnanda[3], Marco Favaro[3,4], Walter Drisdell[3,4], Zahid Hussain[3], Bruce S. Brunschwig[1], Zhi Liu[3,5,6], Nathan S. Lewis[1,2], and Hans-Joachim Lewerenz[1,2] — [1]Caltech, Pasadena, USA. — [2]JCAP, Pasadena, USA. — [3]LBNL, Berkeley, USA. — [4]JCAP, Berkeley, USA. — [5]Chinese Academy of Sciences, China. — [6]ShanghaiTech University, China. — [7]BTU C-S, Cottbus, Germany.

The performance of a photoelectrochemical solar cell depends strongly on the electrochemical nature of the semiconductor/electrolyte junction [1]. Operando Ambient Pressure X-ray photoelectron spectroscopy investigation of semiconductor/liquid junctions provides quantitative understanding of the energy bands in these photoelectrochemical solar cells [2, 3, 4]. We demonstrate how OAP-XPS may be used to determine these relationships for semiconductor/liquid systems. The data can be analyzed to determine the energy relationship between the electronic energy bands in the semiconductor electrode and the redox levels in the solution. The major conditions for semiconductor-electrolyte contacts including accumulation, depletion, and Fermi-level pinning are observed, and the so-called flat-band energy can be determined. [1] Science 344 (2014) 1005; [2] Sci Rep 5 (2015) 9788; [3] Ener & Env Sci 8 (2015) 2409; [4] J Electrochem Soc 162 (2016) H1

O 73: Surface Dynamics: Reactions and Elementary Processes

Time: Wednesday 18:15–20:30 Location: Poster A

O 73.1 Wed 18:15 Poster A

Near-ambient pressure XPS study of Pt-Ga alloys and their oxidation — •Mathias Grabau[1], Sandra Krick Calderon[1], Florian Rietzler[1], Nicola Taccardi[2], Peter Wasserscheid[2], Florian Maier[1], Hans-Peter Steinrück[1], and Christian Papp[1] — [1]Physikalische Chemie 2, FAU Erlangen — [2]Chemische Reaktionstechnik, FAU Erlangen

Alloys of 0.7 and 1.8 at.% Pt in Ga and their oxidation were probed by XPS. The Pt surface concentration of metallic alloys was determined as a function of temperature: A constant Pt concentration was observed at high temperature. Phase separation, that is, the formation of a solid Ga_6Pt phase submerged in a Pt-depleted liquid phase, is indicated by a systematic decrease in Pt content at temperatures below 700 and 800 K, respectively. Exposure of the liquid-gas interface of such two-phase systems to oxygen at pressures between $3 * 10^{-7}$ and 1 mbar and at temperatures between 300 and 550 K led to the formation of Pt-enriched Ga_2O_3 films on the surface. Growth and composition of the formed films were examined in- and ex situ as a function of temperature and pressure. Within the examined parameter space, Pt concentration in the formed films is found to be independent of the bulk Pt concentration, growth and thickness of the films. This indicates defined solubility of Pt in Ga_2O_3 or the formation of discrete structural motives during oxidation.
We acknowledge the support of the Cluster of Excellence 'Engineering of Advanced Materials'.

O 73.2 Wed 18:15 Poster A

CO oxidation on TiO_2 nanotube-supported Pt particles at near ambient pressures — •Sandra Krick Calderon[1], Mathias Grabau[1], Jeong Eun Yoo[2], Patrik Schmuki[2], Hans-Peter Steinrück[1], and Christian Papp[1] — [1]Physikalische Chemie II, University of Erlangen-Nürnberg, Egerlandstr. 3 — [2]Lehrstuhl für Korrosion und Oberflächentechnik, University of Erlangen-Nürnberg, Martensstraße 7, 91058 Erlangen, Germany

We investigated the oxidation of CO on different platinum model catalysts, i.e., differently sized Pt particles on vertical TiO_2 nanotubes (d=80, l=100 nm); the results are compared to the behaviour on a TiO_2(110) rutile crystal with a similar Pt content and a Pt(111) single crystal. Temperature-programmed reaction experiments at total pressures of 1.0 and 0.1 mbar, and a CO:O_2 ratio of 1:4 and 2:1, were examined by near-ambient pressure XPS in the temperature range from 300 to 800 K. Additionally, we performed online gas analysis. The onset temperature of the reaction on the Pt/TiO_2 nanotube samples was found to be lower than on Pt(111) and Pt/TiO_2(110) and to decrease with decreasing particle size. After reaction onset no adsorbed CO was found on the particles and metallic platinum was the active catalyst. Strong ageing of the TiO_2-supported samples with reaction time was observed resulting in changes of the reaction onset and CO conversion. Further measurements to elucidate the role of UV light for the enhancement of the reactivity will be discussed. The work was supported by Cluster of Excellence "EAM" of the Friedrich-Alexander-Universität.

O 73.3 Wed 18:15 Poster A

In-situ UPS and high-resolution XPS investigations on the norbornadiene/quadricyclane energy storage system on different metal substrates — •Udo Bauer, Philipp Bachmann, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Germany

Fossil fuel-based energy technologies lack a long-term perspective. The further development of existing renewable energy concepts is needed regarding energy distribution and storage. One possible scenario is the storage of energy by chemical means in the form of strained organic molecules, e.g. the multi-cyclic hydrocarbon quadricyclane (QC) and its strain-released counterpart norbornadiene (NBD). By absorption of light, NBD is transformed to the energy rich QC, followed by a catalytic energy release to reform NBD. We investigated the adsorption as well as the conversion of QC to NBD and their decomposition over different catalytically active metal surfaces. Ultraviolet photoelectron spectroscopy (UPS) provides characteristic spectra of NBD/QC on Ni(111) and Au/Ni(111) but not on Pt(111). By applying heating ramps, we observe the conversion of QC to NBD at certain temperatures except for the Pt(111) surface, where the reaction takes place below 120 K. HR-XPS (high-resolution X-ray photoelectron spectroscopy) spectra of the adsorption (120 K) and during the heating ramps reflect the different interaction strength between molecules and surface and reveal a fundamentally changed decomposition behavior of NBD at higher temperatures for each surface. The work was supported by the Cluster of Excellence Engineering of Advanced Materials (EAM).

O 73.4 Wed 18:15 Poster A

XPS Characterization of Sulphur Transformations during Operation of Li-S Batteries with Ultramicroporous Carbon-Sulphur Cathodes — •Thomas Diemant[1], M. Helen[2], M. Anji Reddy[2], Maximilian Fichtner[2,3], and R. Jürgen Behm[1,2] — [1]Institute of Surface Chemistry and Catalysis, Albert-Einstein-Allee

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Lithium-sulphur (Li-S) batteries are discussed as potential successors of Li-ion cells. However, mainly due to the 'poly-sulphide shuttle', Li-S batteries suffer at present from poor cycle life. One promising approach to overcome this problem is the use of microporous carbon confined sulphur, which eliminates the formation of higher order poly-sulphides. In this study, electrodes based on an ultramicroporous carbon-sulphur (UC-S) composite (46% S) were investigated. We studied the chemical state of sulphur in the UC-S cathodes at different stages of the lithiation/delithiation cycle by XPS analysis of the surface and subsurface region of the electrodes. Reasons for the capacity fading over cycling of the UC-S electrodes were elucidated. The structural properties were revealed using transmission electron microscopy (TEM). The results of XPS analysis together with the electrochemical performance measurements demonstrate the single step transformation of sulphur to Li_2S_2/Li_2S and vice versa during the discharge/charge process. The UC-S electrodes used in this study exhibited a reversible capacity of 700 mAh/g at C/5 even after 100 cycles.

O 73.5 Wed 18:15 Poster A

Controlling Alkyne Catalysis on an Atom-By-Atom Basis

— Marian D. Rötzer, Andrew S. Crampton, •Maximilian Krause, Florian F. Schweinberger, and Ueli Heiz — Technische Universität München, Dept. of Chem. and Catalysis Research Center, Chair of Physical Chemistry, Lichtenbergstr. 4, 85748 Garching, Germany

Alkanes, alkenes and alkynes are major feedstocks for the chemical industry and their reactions on supported metal nanoparticles are applied in a variety of processes for the synthesis of important chemicals. To be able to develop new and efficient catalysts for those reactions a deep fundamental understanding with respect to adsorption, mechanistic details, poisoning, etc. has to be gained. Size-selected clusters supported on thin films under UHV conditions meet the requirements of a defined model system for unraveling underlying catalytic principles. To this end, we investigated the surface chemistry of 3-hexyne on size-selected Pt_n clusters on MgO(100)/Mo(100). This model system is characterized by TPR and IRRAS and compared to the Pt(111) surface. Depending on the cluster size, different reaction pathways are favored or even completely blocked. The selectivities towards such pathways are size-dependent, though not linearly. IRRAS experiments showed re-emerging free surface sites when the reaction products are desorbed, though a characteristic red-shift of the CO-stretch signal points to the remainder of carbonaceous species, as supported by AES.

This work has been supported by the Clariant Produkte (Deutschland) GmbH in the framework of the Munich Catalysis (MuniCat) program, a strategic alliance between TUM and Clariant.

O 73.6 Wed 18:15 Poster A

STM Tip-Induced Manipulation of Tetrahydrofuran and Diethyl Ether on Si(001)

— •Tamam Bohamud[1], Marcel Reutzel[1], Gerson Mette[1], Michael Dürr[1,2], and Ulrich Höfer[1] — [1]Philipps-Universität, 35037 Marburg — [2]Justus-Liebig Universität, 34392 Gießen

In the last decades, the adsorption of organic molecules on silicon surfaces has been subject of intense research. The resulting hybrid structures provide a promising tool to increase the functionality of semiconductor devices. In most cases, the respective adsorbate reactions are thermally induced; however, electronically induced processes may open additional reaction pathways and/or better control of single reaction channels. In this study, we investigate both lateral movement as well as chemical conversion of ether molecules on Si(001) induced by tunneling electrons from a STM tip.

The adsorption mechanism of ether molecules on Si(001) is well understood: At low temperature, a dative bond between the oxygen atom of the intact ether molecule and the D_{down} state of the buckled silicon dimer is established. At room temperature, ether cleavage leads to covalent Si-O and Si-C bonds [*ChemPhysChem* **15**, 3725 (2014), *JPCC* **119**, 6018 (2015)]. For Diethyl Ether, a tip-induced hopping of a $-C_2H_5$ fragment is observed at positive sample bias. For Tetrahydrofuran, the tunneling electrons can induce the transition from the datively bonded intermediate state to the covalently bonded final state. In both cases, we observe a dependence on tunneling voltage and current which are discussed in terms of the underlying excitation mechanism.

O 73.7 Wed 18:15 Poster A

A transition metal complex transformation in ionic liquids monitored by photoelectron spectroscopy

— •Benjamin May, Michael Hönle, Hans-Peter Steinrück, and Florian Maier — Chair Physical Chemistry II, FAU University Erlangen-Nürnberg, Germany

Ionic liquids (ILs) — salt melts with melting points below 373 K do exhibit an extremely low vapor pressure making them suitable for surface science investigations under ultra-high vacuum conditions, in contrast to conventional molecular liquids. Within the last years, our group performed various types of fundamental reaction studies in ILs in combination with X-ray photoelectron spectroscopy (XPS).[1] Here, we report on a temperature-dependent IL metal complex transformation.

The transition metal IL $[EMIM]_2[Co(NCS)_4]$[2] was mixed with the IL [EMIM][NCS]. Osborne *et. al.* reported thermochromic behavior for a similar system: in the presence of an excess of free thiocyanate anions, the blue tetrahedral $[Co(NCS)_4]^{2-}$ complex anion reversibly forms below 223 K a pink octahedral $[Co(NCS)_6]^{4-}$ complex.[3]

In our study, IL signals were monitored by XPS and UPS between room temperature and 213 K. Below the transition temperature, changes in the Co2p line were observed indicating a shift of the complex equilibrium towards the octahedral complex.

[1] H.-P. Steinrück, Phys. Chem. Chem. Phys. 2012, 14, 5010-5029.
[2] T. Peppel, et. al., Angew. Chem. Int. Ed. 2010, 49, 7116-7119.
[3] S.J. Osborne, et. al. , Dalton Trans. 2015, 44, 11286-11289.

O 73.8 Wed 18:15 Poster A

Theoretical model for the time evolution of a diffusion grating at a solid-liquid interface

— Alexandra C. Dávila[1], •Eckhard Pehlke[1], Daniel Beicht[2], and Olaf Magnussen[2] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

Diffusion at electrochemical interfaces is a fundamental process in electrochemistry. It is the crucial factor determining, e.g., the growth mode during electrolytic deposition and thus, ultimately, the quality of the deposited films. Under UHV conditions, surface diffusion coefficients have been measured by various techniques [see, e.g., J.V. Barth, Surf. Sci. Rep. **40**, 75 (2000)], for instance by analyzing the evolution of adsorbate concentration profiles on the surface. Here we go beyond the situation in UHV and present a mathematical model for the time evolution of the concentration profile of a concentration grid at a solid-liquid interface created by Laser induced thermal desorption. The desorption of particles from the adsorbate layer into the liquid, the diffusion in the liquid, and the adsorption back onto the surface are accounted for. The effect of diffusion of the adsorbate through the liquid will be discussed.

O 73.9 Wed 18:15 Poster A

Electrochemical etching of proton irradiated p-GaAs

— •Alrik Stegmaier, Ulrich Vetter, and Hans Hofsäss — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Microelectromechanical systems (MEMS) combine electrical and mechanical features on the micrometer scale and are used for an increasing number of applications, including energy harvesters, accelerometers and pressure sensors [1]. Proton beam writing (PBW) is a maskless lithographic method for the production of microstructures for such applications [2]. With PBW it is possible to produce three dimenstional structures by varying only the fluence of the proton irradiation on a p-GaAs sample, followed by electrochemical etching [3].

As such, the electrochemical etching of the sample is of large importance for producing high quality final structures. While electrochemical etching of defect poor GaAs is reasonably well understood [4] there is comparatively little published work on highly irradiated material.

Here the electrochemical etching with KOH of p-GaAs irradiated with protons (energies up to several MeV) is investigated experimentally, improving upon previous findings [5].

[1] V. Cimalla et al., J. Phys. D: Appl. Phys., 40(20), 6386, 2007
[2] J.A. van Kan et al., Appl. Phys. Lett., 83(8), 1629, 2003
[3] P. Mistry et al., Nucl. Instr. Meth. Phys. Res. B, 237, 188, 2005
[4] P. Allongue et al., J. Electroanal. Chem., 317, 77-99, 1991
[5] M. Schulte-Borchers et al., J. Micromech. Microeng., 22, 025011, 2012

O 73.10 Wed 18:15 Poster A

Investigation of Calcium-Silicate surfaces with UHV-IRRAS to understanding the first step in the corrosion of concretes

— •Carsten Natzeck, Peter Weidler, Christof Woell, and Peter Thissen — Institute of Functional Interfaces, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

The well-oriented Calcium-Silicate substrate Wollastonite as our model sample is a chemically well characterized mineral ($CaSiO_3$). It has versatile physical properties for use in industry, reaching from medicine with the formation of artificial bones due to its bioactivity to construction chemistry with Calcium-Silicates (CS) as model system e.g. for cement and concrete. The surface chemistry of this CS substrate has been studied using infrared reflection-absorption spectroscopy under ultrahigh-vacuum conditions (UHV-IRRAS) using water and methanol as probe molecules. Exposure of the cooled substrate (100 K) to H_2O leads to the formation of surface OH-species. This proton transfer, which is a crucial step in the corrosion of concrete, is found to be absent when the same surface is exposed to methanol. These results are analyzed on the basis of a detailed, first-principles computational study employing densitiy function theory (DFT) and allow to derive a consistent picture on the chemical properties of this important mineral surface. Implications for corrosion protection of concrete in harsh environments will be discussed.

O 73.11 Wed 18:15 Poster A

Molecular Level Understanding of the Sorption of the Phosphorus-Containing Compounds on Mineral Surfaces — •Ashour Ahmed and Oliver Kühn — Institute of Physics, University of Rostock, Rostock, Germany.

The future of universal supply with phosphorus (P) fertilizer has got a critical attention that alarmed the public research platforms and also initiated novel ones. Improvement of our understanding to the soil P cycle needs advances in analytical and theoretical methods of investigation. In the current contribution, we are going to explore the optimal quantum-chemical strategy to describe P-related processes at soil mineral surfaces. Since P exhibits a great diversity of inorganic and organic P species, we investigate the different binding motifs and energies of these species at different mineral surfaces using density functional theory. Particular attention is paid to unravel the competition between P- and organic compounds for mineral surface sites in the presence of water.

O 73.12 Wed 18:15 Poster A

Adsorption and diffusion of cobalt phthalocyanine molecules on the Ag(100) surface — Grazyna Antczak[1], •Wojciech Kamiński[1], Agata Sabik[1], Christopher Zaum[2], and Karina Morgenstern[3] — [1]Institute of Experimental Physics, University of Wrocław, Wrocław, Poland — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [3]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, Bochum, Germany

Surface diffusion is essential to many technological processes, such as crystal growth, catalysis, sintering, etc. It influences the stability of functional and technologically important materials. The surface diffusion of adatoms on surfaces has been already widely investigated, but it is still the remaining challenge to probe and fully understand the motion of bigger objects, such as organic molecules.

We investigate the geometry, the electronic structure, and the diffusion mechanism of CoPc molecules adsorbed on the Ag(100). The measurements were performed using the LT-STM and supported with the DFT calculations. We demonstrate that the complex surface diffusion mechanism of CoPc molecules involves, in the same temperature range, a combined translational and rotational molecular motion. Both processes are associated with similar activation energies; however, the translation is more frequently observed. Two channels for surface diffusion were identified: the first provides only a channel for translation, while the second couples the translational and the rotational molecular motion on the transition path. The existence of the two channels explains a higher rate for the translation determined in experiment.

O 73.13 Wed 18:15 Poster A

Pt single atoms and nanoclusters stabilized by ultrathin oxide film: performance and oxygen vacancy creation in CO oxidation — •xiong zhou[1,2], kai wu[1], and wei chen[2] — [1]BNLMS, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China — [2]Department of Chemistry, National University of Singapore, Singapore 117543, Singapore

A series of model catalysts consisting of Pt single atoms and nanoclusters supported by monolayered CuO film grown at Cu(110) were successfully prepared, which could be stabilized well above room temperature and exhibited a high performance in CO oxidation at temperatures as low as ~360 K. Combined scanning tunneling microscopy and temperature-programmed desorption measurements directly evidenced that at the initial CO oxidation stage, oxygen vacancy in the CuO lattice was generated at the nearest neighbour of the Pt nanoclusters. The experimental measurements showed that the oxidation activity was inversely proportional to the Pt nanocluster size. In contrast, the Pt single atoms possessed no surface reactivity for the CO oxidation due to the early and complete desorption of CO before its oxidation on the model catalysts commenced.

O 73.14 Wed 18:15 Poster A

Photon Induced Processes in CH_4:D_2O Interstellar Ice Mimics Initiated by Femtosecond XUV Pulses — •John Thrower, Tushar Suhasaria, Robert Frigge, Sebastian Roling, and Helmut Zacharias — Physikalisches Insitut, Westfälische Wilhelms-Universität Münster, Münster, Germany

Solid state physical and chemical processes on dust grain surfaces play an important role in the chemical evolution of the interstellar medium. In dense molecular clouds, these grains are coated with layers of H_2O dominated molecular ices doped with carbon containing species including CO, CH_3OH and CH_4. Star formation can lead to these ices being bathed in a flux of XUV and soft X-ray photons, providing a non-thermal energetic input that can lead to the production of more complex species as well as providing a low temperature desorption route for returning molecules to the gas phase. We have used femtosecond XUV (λ = 30.4 nm) pulses generated by the Free-Electron Laser in Hamburg (FLASH) to irradiate interstellar ice mimics consisting of D_2O and CH_4 deposited on an HOPG substrate at 15 K. Time-of-flight mass spectrometry, combined with multiphoton ionisation, reveals a rich variety of neutral and ionic desorption products including ejected ionic clusters. The ion desorption yield is found to be non-linear with respect to the photon flux, permitting the probing of reaction dynamics using two correlated pulses, temporally separated by 0.5-6 ps.

O 73.15 Wed 18:15 Poster A

XUV photochemistry of CO and $^{13}CD_3OD$ ice mixtures on HOPG — •Tushar Suhasaria, John Thrower, Robert Frigge, Sebastian Roling, and Helmut Zacharias — Physikalisches Institut, Universität Münster, Germany

In the interstellar medium (ISM), photochemical reactions occur on the surface of dust grains. In cold regions the grains are covered by mixed molecular ices. In these ice matrices, high-energy radiation from young stars leads to the formation of new molecules. On a cold (*ca.* 15 K) highly-oriented pyrolytic graphite (HOPG) surface, a mixture of CO and $^{13}CD_3OD$ was irradiated by 30.4 nm femtosecond XUV pulses from the Free-electron laser in Hamburg (FLASH). The resulting desorption products were identified by time-of-flight mass spectrometry and are dominated by low mass fragment ions from the adsorbed molecules along with some higher mass clusters. In addition, a (2+1) resonance enhanced multi-photon ionization (REMPI) scheme via the $B^1\Sigma \leftarrow X^1\Sigma$ transition of CO molecules at 230 nm was used to probe the internal energy content of desorbing neutral CO. The desorbing ions and neutral products show a non-linear intensity dependence which allows the determination of the reaction dynamics by two-pulse correlation measurements.

O 73.16 Wed 18:15 Poster A

Ultraschnelle Dynamik von Photooxidationsreaktionen auf Titandioxid — •Florian Knall und Thorsten Bernhardt — Universität Ulm

Titandioxid ist ein wichtiger Photokatalysator, dessen Einsatzbereiche von der Entfernung organischer Schadstoffe in der Umgebungsluft über Abwasser-Aufbereitung bis hin zu selbstreinigenden Oberflächenbeschichtungen reichen. Die Photooxidation von organischen Molekülen ist in all diesen Bereichen von Bedeutung. Allerding sind in vielen Fällen sehr wenige molekulare Details der oft hochkomplexen Reaktionen bekannt. Ein molekulares Verständnis der elementaren Reaktionsschritte bildet jedoch die unbedingte Voraussetzung zur gezielten Optimierung moderner photokatalytischer Materialien. Wir verwenden eine neue experimentelle Methode, die Oberflächen-Pump&Probe-Laser-Massenspektrometrie, welche ideal geeignet ist, um derartige Reaktionen zu untersuchen. In diesem Beitrag wird diese neue Technik auf die Photooxidation organischer Adsorbate auf Titandioxid angewendet, um so erstmalig einen Einblick in die elementaren molekularen

Reaktionsdetails photokatalytischer Reaktionen an Oxidoberflächen zu erhalten.

O 73.17 Wed 18:15 Poster A

Pump-probe photoemission spectroscopy of O_2 on Pt(111) at a Free-Electron Laser — •Giuseppe Mercurio[1], Lukas Wenthaus[1], Florian Hieke[1], Henrike Hümpel[1], Günter Brenner[2], Harald Redlin[2], and Wilfried Wurth[1,2] — [1]Physics Department and Center for Free-Electron Laser Science, University of Hamburg, Hamburg, Germany — [2]DESY Photon Science, Hamburg, Germany

The interaction of oxygen with the platinum surface has been the subject of extensive experimental and theoretical studies in the last decades because of its technological relevance in many catalytic reactions. In order to improve heterogeneous catalysis at surfaces to achieve more efficient catalysts and less undesired by-products it is essential to gain a microscopical understanding of fundamental chemical reactions. To this purpose we investigate chemisorbed oxygen molecules on a Pt(111) surface by means of time-resolved photoemission spectroscopy in a pump-probe experiment. We used as pump fs laser pulses at 800 nm and as probe free-electron laser pulses from FLASH at DESY in Hamburg at 566 eV. In this way the dynamics of the adsorbed molecule and the energy exchange with the surface leading to the excitation of the adsorbates could be investigated with a time resolution better than 500 fs for several ps after the absorption of the pump pulse at the surface.

O 74: Ultrafast Electron and Spin Dynamics at Interfaces

Time: Wednesday 18:15–20:30 Location: Poster A

O 74.1 Wed 18:15 Poster A

Electron dynamics at an azobenzene-functionalized metal surface — Wibke Bronsch, Larissa Boie, •Cornelius Gahl, and Martin Weinelt — Fachbereich Physik, Freie Universität Berlin, Germany

Self-assembled monolayers (SAMs) of azobenzene-decorated alkanethiols represent a versatile class of systems for the functionalization of a metal surface with molecular switches. The alkyl-linker chains serve as a buffer layer to efficiently decouple the chromophores from the metal substrate. In this contribution we investigate the electron dynamics in SAMs of azobenzene-decorated undecane thiol diluted with dodecanethiol on Au(111) by means of two-photon photoemission spectroscopy. For a pure dodecanethiolate SAM a lifetime of ∼50 ps has been reported for an image potential state [1]. We found that the presence of azobenzene shortens its lifetime considerably. Furthermore, photoisomerization causes a change of the work function depending on the density of the photochromic moieties.

[1] M. Shibuta, N. Hirata, R. Matsui, T. Eguchi, and A. Nakajima, J. Phys. Chem. Lett. 3, 981 (2012).

O 74.2 Wed 18:15 Poster A

Exciton Dynamics in Thin Sexithiophene Films on Au(111) — Wibke Bronsch[1], •Sebastian Baum[1], Malte Wansleben[1,2], Kristof Zielke[1], Cornelius Gahl[1], and Martin Weinelt[1] — [1]Freie Universität, Berlin, Deutschland — [2]Physikalisch-Technische Bundesanstalt, Berlin, Deutschland

Sexithiophene (6T)/Gold is a model system for an organic semiconductor/metal interface. Exciton formation and relaxation as well as charge transfer processes across those interfaces are of high relevance in molecular electronics. Starting from the optical properties of thin 6T films on Au(111) investigated by differential reflectance spectroscopy, we performed time-resolved two-photon photoelectron spectroscopy using different excitation energies below and within the vibrational progression of the S1 absorption band. As a result we can draw a detailed picture of the exciton dynamics.

O 74.3 Wed 18:15 Poster A

High harmonic generation at 500 kHz: an XUV light source for solid state spectroscopy — •Johannes Feldl, Michele Puppin, Yunpei Deng, Martin Wolf, and Ralph Ernstorfer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin

We present a table-top ultrafast extreme ultraviolet (XUV) light source operating at a repetition rate of 500 kHz. The frequency-doubled output of an optical parametric chirped pulse laser amplifier drives high harmonic generation (HHG) in noble gas jets with high backing pressure. A single harmonic with photon energy near 22 eV and a bandwidth of 100 meV is spectrally isolated. The best photon flux, exceeding 10^{11} photon/s from HHG, was obtained with an argon gas jet. This high-repetition rate XUV light source permits time- and angle-resolved photoemission spectroscopy with high counting statistics and provides access to electron dynamics in the full Brillouin zone.

O 74.4 Wed 18:15 Poster A

Resonant excitation and circular dichroism of the second Dirac cone of the topological insulator Bi_2Se_3 — •Sophia Ketterl[1], Sebastian Otto[2], Martin Bastian[1], Cornelius Gahl[1], Thomas Fauster[2], and Martin Weinelt[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

Topological insulators (TIs) host metallic topological surface states (TSS) with helical spin structure. This makes them promising materials for the generation of spin-polarized currents. The TI Bi_2Se_3 is intrinsically n-doped and thus the TSS at the Γ point with a Dirac cone dispersion is occupied. Two-photon photoemission (2PPE) experiments have shown that Bi_2Se_3 exhibits a second Dirac cone in the band gap between the second and third conduction band [1].

We studied the properties of the second Dirac cone of Bi_2Se_3 by 2PPE with both linearly and circularly polarized light. We show that the second Dirac cone can be populated directly from the first Dirac cone by photoexcitation with 1.7 eV photon energy. We observe dichroic photoemission for both circularly polarized probe and pump pulses. This hints at a helical spin structure of the second Dirac cone [1] and its asymmetric population, respectively. Both are necessary to create photocurrents with a definite spin polarization.

We studied the temporal evolution of the transient population of the second Dirac cone in order to understand how inter- and intraband scattering influences photocurrents within the TSS.

[1] D. Niesner *et. al.*, *Phys. Rev. B* **86**, 205403 (2012).

O 74.5 Wed 18:15 Poster A

Investigation of charge dynamics by optical Pump-Probe Scanning Tunneling Microscopy — •Terence Thias, Philipp Kloth, Katharina Kaiser, and Martin Wenderoth — IV. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The combination of optical Pump-Probe techniques with Scanning Tunneling Microscopy (STM) enables us to merge atomic resolution of an STM with time resolution on the ns time scale. As it is beyond the bandwidth of the current amplifier we use Shaken-Pulse-Pair-Excitation technique [1]. By illuminating the n-doped GaAs(110) surface we generate electron hole pairs, which will be separated in the tip-induced Space Charge Region (SCR). This results in a hole accumulation layer at the surface. As recent results have shown [2] these holes can serve as an additional tunnel channel into the valence band. Studying the time evolution of the photo-induced tunnel current gives access to the charge dynamics .Surprisingly, we have found a dependency on the pulse duration of excitation as well as on the tunnel current. We discuss two main processes determining the relaxation characteristic of the excited system. One process is the filling of the photo-generated holes trapped at the surface, the other is the charging/discharging of dopants changing the local SCR beneath the STM tip.

[1] Terada et al., Nature Photonics, 4(12), 2010

[2] Kloth et al., Nat. Comm. (2015)

O 74.6 Wed 18:15 Poster A

A setup for time-resolved SHG microscopy of 2D heterostructures — •Jonas Zimmermann, Gerson Mette, and Ulrich Höfer — Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

Van-der-Waals coupled 2D materials span the whole range from metallic over semiconducting up to isolating materials and their combination leads to fascinating opportunities for designing stacked heterostructures. The huge variety of possibilities calls for experimental methods which can effectively probe the structure as well as the electron dynamics of these heterostructures.

Here, we present an experimental setup for time-resolved studies on interfaces of 2D heterostructures by means of SHG microscopy. This technique allows us to quantify the crystal structure via polarization dependent measurements and will give access to the electron dynamics via time-resolved pump-probe measurements. We demonstrate the capabilities of our setup with measurements done on CVD grown polycrystalline WS_2 monolayer flakes. The resolution of the experiment is diffraction limited to about 2μm. The relative orientation of several crystal domains can be determined with an error of a few degrees. Because the setup is designed to exclude any dispersion afflicted components, high temporal resolution by the use of ultra-short laser pulses in a pump-probe measurement is feasible. This combination of high temporal and spatial resolution can be applied to 2D heterostructures to study the effects of relative crystal orientation on time-dependent charge transfer processes between different materials.

O 74.7 Wed 18:15 Poster A

Mutual influence of relaxation processes in laser-irradiated metals — •Kai Klein, Sebastian Weber, and Baerbel Rethfeld — Fachbereich Physik und Forschungszentrum OPTIMAS, TU Kaiserslautern, Germany

When an ultrashort laser pulse irradiates a metal, energy is absorbed by the electron system which is driven out of thermal equilibrium on a femtosecond time scale. Due to electron-electron collisions a new thermodynamical equilibrium state within the electron system is established in a characteristic time, the so-called thermalization time. At the same time, electron-phonon collisions transfer energy to the phononic system until both temperatures equilibrate.

We study the dynamics of the nonequilibrium systems by applying complete Boltzmann collision integrals to describe the transient electron distribution due to excitation, thermalization and relaxation. Specific material properties enter the calculation through the density of states.

The results show the mutual influence of both collision processes. We see that the coupling to the phonons affects the electron thermalization. Moreover, the electron-phonon coupling strength differs from the equilibrium coupling, when the electron system is not thermalized.

O 75: Overview Talk: Ulrike Diebold

Time: Thursday 9:30–10:15 Location: S054

Invited Talk O 75.1 Thu 9:30 S054

Ternary oxides with the perovskite structure exhibit an intriguingly rich variety in their physical and chemical properties. — •Ulrike Diebold — Institute of Applied Physics, TU Wien, Wiedner Hauptstrasse 8-10/134, 1040 Vienna, Austria

The surfaces of these promising, yet complex materials are poorly understood. In the talk I will provide an overview of surface studies of perovskite oxides, and, for a few examples, discuss optimum preparation parameters for a reproducible surface structure and how this affects reactivity and growth.

The surface of $Sr_3Ru_2O_7$, the n=2 member of the Ruddlesden-Popper series, is structurally quite simple: cleaving in UHV yields a SrO-like top layer, which is essentially defect-free, except for impurities in the bulk material. The surface is very reactive towards components of the residual gas, however. CO, CO_2, and H_2O adsorb readily and form adsorption complexes. $SrTiO_3(110)$ is polar and exhibits a series of reconstructions that can be controlled by adjusting the chemical potential of its constituents, i.e. by evaporating appropriate amounts of Sr and Ti and annealing in O_2. The (n×1) reconstructions consist of a monolayer of titania with tetrathedrally-coordinated Ti atoms that are arranged in corner-sharing rings. When the Ti chemical potential is increased, the surface switches over to a (2×m) symmetry with a titania layer that is composed of Ti in octahedral coordination. These stoichiometry-dependent, facile structural changes have a profound effect on surface reactivity, and on the homoepitaxial growth of $SrTiO_3$ during pulsed laser deposition.

O 76: 2D Materials beyond Graphene: Dynamics and Excitation

Time: Thursday 10:30–13:30 Location: S054

Invited Talk O 76.1 Thu 10:30 S054

Spin- and Pseudospin-Polarized Excited States in bulk WSe_2 — Roman Bertoni[1], Christopher Nicholson[1], Lutz Waldecker[1], Michele Puppin[1], Claude Monney[2], Cephise Cacho[3], Hannes Huebener[4], Umberto De Giovannini[4], Angel Rubio[4], Martin Wolf[1], and •Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]University of Zurich, Zurich, CH — [3]Rutherford Appleton Laboratory, Didcot, UK — [4]University of the Basque Country, San Sebastian, ES

The peculiar electronic structure of layered semiconducting transition metal dichalgogenides (TMDC) like WSe_2 gives rise to internal quantum degrees of freedom of the electrons in addition to the spin, namely valley and layer pseudospins. Employing XUV-based time- and angle-resolved photoemission spectroscopy (trARPES) with resonant excitation of excitonic transitions, we observe circular dichroism in the excited state population in the K valleys of the topmost trilayer of bulk WSe_2. Such spin-, valley and layer-polarized excitations are a manifestation of broken site symmetry in an inversion-symmetric crystal. The valley- and layer-resolved view on excited state dynamics provided by trARPES is complemented by the investigation of electron-lattice coupling in multilayer WSe_2 with femtosecond electron diffraction. Latter studies reveal the dynamics of global energy transfer from electronic to vibrational degrees of freedom in TMDCs subsequent to excitonic as well as interband excitation.

O 76.2 Thu 11:00 S054

Exciton dynamics in two-dimensional materials with strong spin-orbit interaction: $MoSe_2$ versus WSe_2 — •Daniel Schmidt[1], Tillmann Godde[2], Johannes Schmutzler[1], Marc Assmann[1], Jörg Debus[1], Freddie Withers[3], Osvaldo Del Pozo-Zamudio[2], Konstantin S. Novoselov[3], Andre Geim[3], Manfred Bayer[1], and Alexander Tartakovskii[2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Department of Physics and Astronomy, University of Sheffield, Sheffield S3 7RH, UK — [3]School of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK

Monolayers of semiconducting transition metal dichalcogenides such as MoS_2, WS_2, $MoSe_2$ and WSe_2 have attracted considerable attention following the discovery of the indirect-to-direct bandgap transition from bulk to monolayer material and the coupling of spin and valley degrees of freedom in atomically thin layers. An important characteristic of these compounds is the strong spin-orbit interaction, which leads to a splitting between dark and bright exciton sub-bands. A detailed understanding of dark and bright exciton dynamics and non-radiative processes is important for light emitting applications as has been demonstrated in other systems such as phosphorescent organic light emitting diodes. We measure time-integrated and -resolved PL in monolayers of $MoSe_2$ and WSe_2 in a wide range of temperatures from 10 to 300K and gain insights into the exciton and trion dynamics. Our study reveals similar carrier dynamics for both materials, whereas pronounced differences have been observed for the overall PL intensities.

O 76.3 Thu 11:15 S054

Electron dynamics in eiptaxial single layer MoS_2 — •Antonija Grubisic-Cabo[1], Jill A. Miwa[1], Signe S. Gronborg[1], Jonathon M. Riley[2], Jens C. Johannsen[3], Cephise Cacho[4], Oliver Alexander[4], Richard T. Chapman[4], Emma Springate[4], Marco

Grioni[3], Jeppe V. Lauritsen[1], Phil D. C. King[2], Philip Hofmann[1], and Soren Ulstrup[1] — [1]Aarhus University, DK — [2]University of St. Andrews, UK — [3]Ecole Polytechnique Federale de Lausanne, CH — [4]CLF, STFC Rutherford Appleton Laboratory, UK

The current understanding of the optical properties and excited carrier dynamics in single-layer and few-layer transition metal dichalcogenides relies largely on a series of photoluminescence and differential absorption measurements. Since excitons dominate the optical response, the dynamics of free carriers cannot be studied directly. Here, we use time- and angle-resolved photoemission spectroscopy to directly measure free carriers in epitaxial single layer MoS_2 grown on either Au(111) or on graphene. For MoS_2/Au(111) we determine an ultrafast (50 fs) extraction of excited free carriers via the metal and ascertain a direct quasiparticle band gap of 1.95 eV. The observed quasiparticle gap is significantly smaller than the theoretically estimated value for free-standing MoS_2. This can be explained by a strong renormalisation of the band gap. For MoS_2 on graphene, we find indications of induced band shifts that lead to a time-dependence of the electronic structure.

O 76.4 Thu 11:30 S054

Understanding optical properties of atomically thin semiconductors from a many-body perspective — •Matthias Drüppel, Thorsten Deilmann, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Transition metal dichalcogenides (TMDCs) open the door to a fascinating, fast growing field of two dimensional atomically thin semiconductors. This increases the demand for novel theoretical techniques, which allow to reliably calculate the optical properties in large systems, the inclusion of substrates or even correlation between more than two particles.

We take the state of the art approach of DFT → GW → Bethe-Salpeter equation (BSE) and apply the efficient LDA+GdW [1] method. This enables us to describe many-body electronic excitations at moderate numerical cost, being able to treat systems of up to 100 atoms. In the LDA+GdW approximation the quasiparticle self-energy corrections result from the difference between the correct semiconducting screening and hypothetical metallic screening.

Our results show how the optical properties of TMDCs are modified in different situations, e.g. when the screening of the substrate is taken into account, in the presence of vacancies, or when three excited particles form a correlated trion state.

[1] M. Rohlfing, Phys. Rev. B. **82**, 205127 (2010)

O 76.5 Thu 11:45 S054

Scanning tunneling light emission from single layer MoS_2 — •Christian Lotze, Nils Krane, Julia Läger, Gaël Reecht, and Katharina J. Franke — FU Berlin, FB Physik, Arnimallee 14, 14195 Berlin

Transition-metal dichalcogenides form a group of interesting 2d materials. Among them, the semiconductor MoS_2 has attracted great interest, because it has been shown that it turns from an indirect-gap into a direct-gap semiconductor when reduced to a single layer [1]. As such, potential applications involve its usage for instance as light emitting device.

Here, we present a combined low temperature scanning tunneling (STM) and light emission (LE) study on MoS_2/Au(111). The STM geometry allows to locally inject electrons or holes with the tip into the single layer MoS_2. Inelastically tunneling electrons and holes can give rise to emission of photons [2,3]. Here, we detect and analyze spectrally resolved the electroluminescence from the MoS_2 monolayer on Au(111). We correlate these LE spectra with the electronic structure, that we obtained from scanning tunneling spectroscopy. Moreover we will look into the spatial variation of the LE signals and the role of defect sites.

[1] Mak *et al.*, PRL 105, 136805 (2010)
[2] Berndt *et al.*, PRL 67, 3796 (1991)
[3] Hoffmann *et al.*, Phys. Rev. Lett. 93, 076102 (2004)

O 76.6 Thu 12:00 S054

Ultrafast photocurrent dynamics in monolayer MoS2 — Eric Parzinger, Anna Vernickel, Alexander Holleitner, and •Ursula Wurstbauer — Walter Schotty Institut and Physik Department, Technical University of Munich, Germany

Atomically thin semiconducting transition metal dichalcogenides such as MoS_2 are emergent materials for optical and electronic circuits. For possible high-frequency applications, we investigate the ultrafast photocurrents in monolayer MoS_2 on a picosecond time scale utilizing a recently developed pump-probe spectroscopy [1-3]. The observed photocurrent contains three major contributions [4]. An initial ultrafast response of $\leq$ 5ps is followed by an exponential decay within a few hundreds of picoseconds. The third very slow contribution peaks at around 1.5 ns. This slow part dominates the overall time-integrated photocurrent intensity. We discuss the impact of laser-induced heating, the one of built-in fields at metal contacts, and the role of trap states. We acknowledge the financial support by the ERC-grant NanoREAL, the DFG excellence cluster Nanosystems Initiative Munich (NIM), and BaCaTec. [1] L. Prechtel, et al. Nature Communications 3, 646 (2012). [2] A. Brenneis, et al. Nature Nanotechnology 10, 135 (2015). [3] C. Kastl, et al. Nature Communications 6, 6617 (2015). [4] E. Parzinger et al. (2016).

O 76.7 Thu 12:15 S054

Electronic excitations in transition metal dichalcogenides under the influence of dielectric environments — •Malte Rösner[1], Alexander Steinhoff[2], Roelof Groenewald[3], Frank Jahnke[2], Stephan Haas[3], Christopher Gies[2], and Tim O. Wehling[1] — [1]Institut für Theoretische Physik and Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany — [2]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [3]Department of Physics and Astronomy, University of Southern California, Los Angeles, CA, USA

We present a material-realistic approach to describe electronic interaction effects in transition metal dichalcogenides. On the basis of the Wannier function continuum electrostatics (WFCE) method [1], we are able to include the effects of the dielectric environment, which could serve as a promising tuning knob to control 2D material's properties. We study the doping dependence and the influence of different types of dielectric environments to electronic and plasmonic properties. We find electronic band structure and plasmon dispersion changes on the eV scale.

[1] M. Rösner et al., Phys. Rev. B 92, 085102 (2015)

O 76.8 Thu 12:30 S054

Optoelectronic properties of sub-nanometer WS2 and TiS3 investigated by scanning near-field optical microscopy and nano-FTIR spectroscopy by using synchrotron radiation — •P. Patoka[1], G. Ulrich[1], A. Nguyen[2], A. Lipatov[3], A. Sinitskii[3], P. Hermann[4], B. Kästner[4], A. Hoehl[4], L. Bartels[2], P. Dowben[5], G. Ulm[4], and E. Rühl[1] — [1]Physikalische Chemie, Freie Universität Berlin, Germany — [2]Dept. of Chemistry, Univ. of California Riverside, U.S.A. — [3]Dept. of Chemistry, Univ. of Nebraska-Lincoln, U.S.A. — [4]Physikalisch-Technische Bundesanstalt (PTB), Germany — [5]Dept. of Physics and Astronomy, Univ. of Nebraska-Lincoln, U.S.A.

Among the 2D electronic materials that have received increased attention recently are the transition metal dichalcogenides (TMD). These materials, especially below nanometer thickness, exhibit promising optoelectronic properties for applications in low-dimension electronic circuits. The combined use of scattering-type near-field optical microscopy and the broadband synchrotron radiation source MLS (PTB, Berlin) allows for the highly sensitive spectromicroscopic characterization of such 2D semiconductors with a spatial resolution below 30 nm. We will present recent results on near-field imaging and nano-FTIR spectroscopy in mid-infrared regime down to monolayer thick TMD structures. Investigated are optical responses of WS2, such as its interaction with the optical phonon mode of the SiO2 substrate. We will also show evidence for high charge accumulation at the edges of the TiS3 structures revealed by optical mapping using tunable CO2 laser.

O 76.9 Thu 12:45 S054

Investigations on the Phonon Spectrum of $TiSe_2$ in the CDW Phase — •Roland Hott, Rolf Heid, and Frank Weber — Karlsruhe Institute of Technology, Institute of Solid State Physics, P.O.B. 3640, D-76021 Karlsruhe, Germany

We report recent results of our investigations on the Charge Density Wave (CDW) phase transition in $TiSe_2$, performed both experimentally by means of high resolution Inelastic X-ray Scattering (IXS) as well as theoretically by Density Functional Theory (DFT) based ab-initio phonon calculations [1].

We extended our calculations to the case of Cu-doping where we found a huge hardening of the CDW-related soft phonon due to strong chemical bonding of the Cu atoms to the TiSe$_2$ host lattice. Moreover, we investigated the phonon spectrum of TiSe$_2$ in the CDW phase where we find the expected stabilisation of the lattice. Nevertheless, we still obtain here a sizeable electron-phonon coupling for the phonons which derive from the soft phonons of the normal (CDW-undistorted) phase.

[1] F. Weber, S. Rosenkranz, J.-P. Castellan, R. Osborn, G. Karapetrov, R. Hott, R. Heid, K.-P. Bohnen, A. Alatas, PRL **107**, 266401 (2011)

O 76.10 Thu 13:00 S054

Ultrafast carrier multiplication in 1*T*-TiSe$_2$ — •Stephan Michael[1], Steffen Eich[1], Henry C. Kapteyn[2], Margaret M. Murnane[2], Michael Bauer[3], Kai Rossnagel[3], Hans Christian Schneider[1], Martin Aeschlimann[1], and Stefan Mathias[4] — [1]University of Kaiserslautern — [2]JILA, University of Colorado and NIST — [3]University of Kiel — [4]University of Göttingen

1*T*-TiSe$_2$ is a transition metal dichalcogenide, which has a charge density wave (CDW) state below a temperature of around 200 K, which may be due to an excitonic insulator mechanism and/or an Jahn-Teller effect. We studied optically excited carrier dynamics on ultrashort timescales in the CDW phase using time-resolved ARPES measurements and an effective two-band model including carrier-carrier Coulomb scattering. In the framework of this model we analyze the ultrafast response of this material to optical excitation, which is seen in the experiment. We show that carrier multiplication in the form of impact ionization is the most satisfactory explanation for the ultrafast redistribution of spectral weight observed in the ARPES measurements.

O 76.11 Thu 13:15 S054

Charge density wave kinetics in 1T-TaS$_2$ monitored by ultrafast LEED — •Simon Schweda[1], Gero Storeck[1], Sebastian Schramm[1], Max Gulde[1], Kai Rossnagel[2], Sascha Schäfer[1], and Claus Ropers[1] — [1]IV. Physikalisches Institut, Universität Göttingen, D-37077 Göttingen — [2]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel

We developed an ultrafast low-energy electron diffraction (ULEED) setup for the study of time-resolved structural dynamics at surfaces, extending our previous approach operating on ultrathin films in transmission [1]. A laser-driven nanometric needle emitter provides well-collimated electron pulses with durations of few tens of ps at the sample for electron energies in the range of 50-200 eV.

In a first application of this technique, we investigate optically induced transitions between charge density wave (CDW) phases [2] at a single-crystalline 1T-TaS$_2$ surface. In particular, the recovery of the nearly commensurate (NC) room-temperature phase after laser-excitation to the incommensurate (IC) phase is resolved in the time-domain. We find a strong dependence of the formation time on the energy density deposited. Furthermore, at higher optical fluences, the appearance of metastable NC antiphase domains is observed, caused by a rapid quench after optical excitation. Our results demonstrate the potential of ULEED for the study of complex ultrafast structural and electronic processes at surfaces.

[1] M. Gulde et al., Science 345, 200 (2014)
[2] M. Eichberger et al., Nature 468, 799 (2010)

O 77: Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00 Location: S051

Invited Talk O 77.1 Thu 10:30 S051

The first single atom magnet — •Fabio Donati[1], Stefano Rusponi[1], Sebastian Stepanow[2], Christan Wäckerlin[1], Aparajita Singha[1], Luca Persichetti[2], Romana Baltic[1], Katharina Diller[1], Edgar Fernandes[1], François Patthey[1], Jan Dreiser[1,3], Željko Šljivančanin[4,5], Kurt Kummer[6], Corneliu Nistor[2], Pietro Gambardella[2], and Harald Brune[1] — [1]Ecole Polytechnique Fédérale de Lausanne — [2]ETH Zurich — [3]Paul Scherrer Institute — [4]Vinča Institute of Nuclear Sciences — [5]Texas A&M University at Qatar — [6]European Synchrotron Radiation Facility

Realizing magnetic remanence in a single atom is the key to store and process information in the smallest unit of matter. To achieve this goal, one needs to protect the magnetic states of the single atom from quantum tunneling of the magnetization and from scattering with the electrons of the supporting substrate. Here we demonstrate that individual rare-earth atoms adsorbed on ultra-thin insulating layers grown on non-magnetic metal substrates exhibit magnetic remanence up to a temperature of 30 K and a relaxation time of 1500 s at 10 K. This first example of a single atom magnet shows bistability at a temperature which is significantly higher than the best single molecule magnets reported so far. Its extraordinary performances are achieved by a suitable combination of magnetic ground state and adsorption site symmetry, as well as by suppressing spin-electron scattering with conduction electrons by ultra-thin insulating layers.

Invited Talk O 77.2 Thu 11:00 S051

When Electron Acceptors Donate Charge: Molecular Orbitals vs Hybrid Bands at Inorganic/Organic Interfaces — •Oliver T. Hofmann[1], Patrick Rinke[2], Matthias Scheffler[3], and Georg Heimel[4] — [1]TU Graz, Graz, Austria — [2]Aalto University, Helsinki, Finland — [3]Fritz-Haber-Insitut der MPG, Berlin, Germany — [4]Humboldt University of Berlin, Germany

At inorganic/organic interfaces, the concept of electrons moving in extended bands collides with the notion of localized molecular orbitals. For the adsorption of most electron accepting molecules, theory and experiment concordantly report an average charge-transfer smaller than one electron per molecule, raising the question how such an (indivisible) object can be divided between the subsystems. Using hybrid density functional theory (DFT) we prepare and contrast both situations for TCNE molecules on clean and NaCl-passivated Cu substrates. Hybrid DFT functionals localize electrons on a subset of individual molecules, who become charged and whose signatures and associated observables differ markedly from the delocalized band states of fractionally charged molecules obtained with semi-local DFT. We then apply our computational framework to F4TCNQ on ZnO(10$\bar{1}$0), which exhibits two different charge transfer types. Charge donation again leads to integer charging of individual molecules, whereas charge back-donation proceeds via covalent bonds and thus delocalized hybrid bands. Since back-donation also occurs for the uncharged F4TCNQ molecules in the organic film, we end up with the counterintuitive situation of positively charged electron acceptors on the ZnO surface.

Invited Talk O 77.3 Thu 11:30 S051

Direct observation of H-bond dynamics using scanning tunneling microscopy — •Takashi Kumagai — Fritz-Haber Institute

H-bond dynamics is involved in many important processes in chemistry and biology. However, it is still poorly understood at the microscopic level because the dynamics, H-bond rearrangement and H-atom (proton) transfer, remains difficult to directly probe at the single-molecule level. Additionally, quantum nuclear effects, like tunneling and zero-point energy, play a crucial role due to the small mass of the H atom, which could cause difficultly in accurately describing the H-bond dynamics. We have used low-temperature STM to directly observe the H-bond dynamics, which were examined with a variety of models assembled from single atoms/molecules by STM manipulation [1-8].

I will discuss the direct observation of several different types of H-bond dynamics; 1) the H-bond exchange reaction governed by tunneling in a water dimer [1], 2) vibrationally-induced H-atom relay reactions in one-dimensional H-bonded water-hydroxyl complexes [4], and 3) the intramolecular H-atom transfer (tautomerization) in a porphycene molecule [6,7]. These results provide a novel insight into H-bond dynamics at the single-molecule level and unveiled the impact of the local environments on the process that is hidden in studies of molecular ensembles probed by spatially-averaging spectroscopies [8].

References; [1] PRL 100, 166101. [2] PRB 79, 035423. [3] PRB 81, 045402. [4] Nat. Mater. 11, 167. [5] Visualization of hydrogen-bond dynamics, Springer (2012). [6] PRL 111, 246101. [7] Nat. Chem. 6, 41. [8] Prog. Surf. Sci. 90, 239.

Invited Talk O 77.4 Thu 12:00 S051

Visualizing topological states of matter and their interaction with perturbations using local probes — •Paolo Sessi — Universität Würzburg

Topological insulators (TIs) are a new class of materials insulating in the bulk but conductive on their surface where they host linearly dispersing gapless Dirac states. The strong spin-orbit coupling perpendicularly locks the spin to the momentum, leads to a chiral spin texture that restricts scattering channels, and results in spin currents intrinsically tied to charge currents. Since all these properties manifest at surfaces, scanning probe techniques are ideal tools to visualize them with both high spatial and energy resolution. In my talk, I will present a series of experiments that allow not only to visualize the presence of Dirac boundary modes, but also to directly prove some of their most remarkable properties. In particular, I will discuss recent efforts focused onto the controlled manipulation of topological states, which is achieved by coupling TIs to well-defined perturbations. First, I will demonstrate that surface magnetic doped TIs can establish magnetic order at very dilute concentrations. Then, I will report on the realization of spin networks of different symmetries conveniently created at TI surfaces by self-assembly processes. Finally, I will illustrate how the introduction of strain can be successfully used to engineer TI transport properties.

Invited Talk O 77.5 Thu 12:30 S051

Surface Chemistry of Oxygen and Water on Anatase TiO_2 (101) — •Martin Setvin[1], Ulrich Aschauer[2], Jan Hulva[1], Michael Schmid[1], Annabella Selloni[3], and Ulrike Diebold[1] — [1]TU Wien — [2]ETH Zurich — [3]Princeton University

TiO_2 is a prototypical material used in photocatalysis, e.g. in water remediation or photocatalytic water splitting. Two polymorphs of TiO_2, rutile and anatase, are used industrially with anatase typically preferred in applications. The surface chemistry of water and oxygen is the basis for majority of (photo)catalytic processes on TiO_2; most prominently in the photocatalytic water splitting and the oxygen reduction reaction. We report adsorption of water and oxygen studied by a combination of experimental and theoretical techniques (STM, nc-AFM, TPD, XPS, DFT). Special attention is paid to the activation of adsorbed O_2 molecules, i.e. electron transfer from the reduced anatase sample to the adsorbate. We show that this can occur in regions with a surplus of excess electrons, e.g., in the vicinity of subsurface donors and at step edges. In other regions the adsorbed O_2 molecules remain neutral. With nc-AFM we show they can be charged by an electron injected from the tip. We find a small energy barrier of 0.3 eV for this process. Interaction between co-adsorbed H_2O and O_2 is used to illustrate the reactivity of thus activated O_2. When the two species react they both dissociate, with terminal $(OH)^-$ groups as the final product of the reaction, stable at room temperature. This species as well as the reaction intermediates, OOH and HOOH, are identified with atomically-resolved SPM measurements.

O 78: Nanostructures at Surfaces IV: Various Aspects

Time: Thursday 10:30–13:00 Location: S052

O 78.1 Thu 10:30 S052

Charge dynamics at semiconductor surfaces investigated with time-resolved Scanning Tunneling Microscopy — •Philipp Kloth, Katharina Kaiser, Terence Thias, and Martin Wenderoth — IV. physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

An overview on the combination of optical excitation and Scanning Tunneling Microscopy (STM) for studying the carrier dynamics at the GaAs(110) surface is given. In this system the tip-induced electric potential is very sensitive to the charge configuration composed of locally fixed dopants and ambipolar optical excited free carriers present at the surface. A detailed spectroscopic analysis [1] has shown that photo-excited charge carriers, trapped in a very local region beneath the STM tip, contribute to the tunneling current. By adjusting the current in a controlled manner we are able to actively access different screening conditions of the electric potential at the surface. Depending on the dominant tunneling channel, pump-probe excitation can resolve different recombination processes of charge in the nanoscaled Space Charge Region. By using the lateral resolution of the STM, the influence of single dopants on the relaxation dynamics of the system is investigated. We discuss the impact of these charged and surface-sided defects in terms of their varying binding energy [2] in comparison to conventional bulk-positioned donors.

[1] Kloth et al., Nat. Comm. (2015) [2] Teichmann et al., PRL (2009)

O 78.2 Thu 10:45 S052

Scanning tunneling potentiometry of resistivity dipoles in thin Bismuth films — •Felix Lüpke, Stefan Korte, Vasily Cherepanov, and Bert Voigtländer — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

We present scanning tunneling potentiometry measurements of thin Bismuth films using a multi-tip scanning tunneling microscope. Defects in the Bismuth films prepared on Si(111) result in localized electric dipoles when a lateral current is injected into the film. We map the potential landscape around such defects and analyze them with respect to classical diffusive transport effects and the Landauer dipole.

O 78.3 Thu 11:00 S052

Circular dichroism and spin polarization from artificial nanostructures — •Daniel Nürenberg[1], Andrew Mark[2], Matthias Kettner[1], Peer Fischer[2], and Helmut Zacharias[1] — [1]Westfälische Wilhelms-Universität, Münster — [2]Max Plank Institut für intelligente Systeme, Stuttgart

Metal nanohelices are receiving growing interest because of their giant plasmon-enhanced optical circular dichroism. We address circular dichroism in multi-photon photoemission from metal nanohelix arrays triggered by polarized ultra-short laser pulses from an optical parametric chirped-pulse amplifier. We use time-of-flight spectroscopy and Mott polarimetry to measure the energy distribution and spin polarization of the emitted electrons. Helices made of non-magnetic Ag:Ti and Ag:Cu alloys on a silicon wafer emit photoelectrons with a polarization dependence in yield and longitudinal spin polarization. The results are compared with single-photon photoemission measurements.

O 78.4 Thu 11:15 S052

Modeling AFM Adhesion Measurements on Rough Substrates — •Till Junge, Michael Schäfer, Christian Greiner, and Lars Pastewka — IAM-CMS, KIT, Karlsruhe, Germany

Understanding adhesion forces in dry contact is of particular importance for the study of both technical and biological micro- and nanoelectromechanical systems. Even in their simplest manifestation – the pull-off force necessary to break the contact between a nano-scale indenter and a rough surface – they are poorly understood. We here use a boundary element method in combination with an empirical interaction potential the contact of a stiff spherical indenter of varying size acting on an elastic rough substrate. The model is compared to a series of atomic-force microscopy (AFM) pull-off measurements performed with silicon tips with tip radii varying between 14 nm and 100 nm on an ultrananocrystalline diamond (UNCD) substrates. Without any fitting parameters, we find good agreement between the experiment and our simulations. We use our simulations to analyze the link between distribution of pull-off forces and statistics of surface roughness of the substrate. This enables in particular extraction of small scale features of the rough topography not accessible by standard AFM measurements, such as the root mean square slope of surface roughness.

O 78.5 Thu 11:30 S052

Morphological study of formation of nanopatterned Si substrate produced by Fe assisted low energy ion beam erosion — •Sarathlal Koyiloth Vayalil[1], Ajay Gupta[2], and Stephan Roth[1] — [1]Photon Science, DESY, Notkestr. 85, D-22607 Hamburg, Germany — [2]Amity Center for Spintronic Materials, Amity University, Sector 125, NOIDA 201313, India

In this work, formation of self-organized Si nanostructures induced by pure Fe incorporation during normal incidence low energy (1keV) Ar+ ion bombardment is presented. It has been observed that the incorporation of Fe affects the evolution of the surface topography. The addition of Fe generates pronounced nano patterns, such as dots, ripples and combinations of dots and ripples. The orientation of the ripple wave vector of the patterns formed is found to be in a direction normal to the Fe flow. The nanoripples with wavelength of the order of 39 nm produced is expected to be the lowest wavelength of the patterns reported on ion beam eroded structures under the incorporation of metallic impurities as per our knowledge. From the AFM and GISAXS analysis, it has been confirmed that the ripples formed are asymmetric in nature. The effect of the concentration of the Fe on morphological transition of the patterns has been studied using Rutherford back scattering measurements.

O 78.6 Thu 11:45 S052

Investigation of thin Ni films on Pd with Positron annihilation induced Auger electron spectroscopy, XPS and STM — •Samantha Zimnik, Christian Piochacz, Sebastian Vohburger, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

Positron annihilation induced Auger Electron Spectroscopy (PAES) is a powerful technique to gather information about the elemental composition of only the topmost atomic layer of a specimen. The positron beam facility NEPOMUC at the research reactor Heinz Maier-Leibnitz in Garching delivers the world's most intense positron beam and enables measurement times of only a few minutes per PAES spectrum. Thus, time-dependent PAES becomes possible and enables the in-situ observation of the surface segregation process. The surface spectrometer at NEPOMUC uses the complementary techniques PAES, X-ray photoelectron spectroscopy (XPS) and Scanning Tunneling Microscopy (STM) to characterize both, the elemental composition of the surface and its topology. Recent studies on sub-monolayers of Ni on Pd using time- and temperature dependent PAES will be presented. Financial support by the BMBF within the project no. 05K13WO1 is gratefully acknowledged.

O 78.7 Thu 12:00 S052

Nanopore-Electrodes With High Aspect-Ratio For High Performance Electrochemical Devices Replicated From AAO-Templates — •Stefan Bösemann, Liaoyong Wen, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau, Germany

Usually nanowires or nanotube arrays are used for high surface area nanostructures. The length of these nanostructures is limited due to agglomeration and collapsing of the NWs or NTs if they reach a specific length. This restricts the reachable aspect-ratio as well as the maximization of the surface area and the device performance. We enhanced a new approach to go beyond this limit with a more stable nanostructure architecture.

Very high aspect-ratios (>100) have been realized with nanopore arrays which show a highly regular structure and made of metal or metal oxides e.g. Ni and NiO2. The fabricated nanopore electrodes can be made of active material or can be utilize as scaffolding for functional core-shell structures for electrochemical devices such as supercapacitors or batteries. The realized devices have the ability to show outstanding performances due to the very high surface area, the highly ordered structure which allows very good ion transport and the conductive metal core which enables a very good electron transfer

O 78.8 Thu 12:15 S052

Chemical characterization and structural evolution of diamond-like carbon films with increasing deposition on polyethylene terephthalate — •Alberto Catena[1], Michael Kunze[2], Simone Agnello[3], Stefan Wehner[1], and Christian B. Fischer[1] — [1]Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany — [2]Department of Chemistry, University Koblenz-Landau, 56070 Koblenz, Germany — [3]Department of Physics and Chemistry, University of Palermo, 90100 Palermo, Italy

The interest in diamond-like carbon (DLC) films on polyethylene terephthalate (PET) steadily increases due to their potential applications as food/beverage packaging and medical devices. Although much is known about the macroscopic features of such composites, the physical and chemical properties of the DLC/PET interface and the film evolution during the deposition are still not fully understood. The films were gradually deposited on PET by radio frequency plasma enhanced chemical vapor deposition with acetylene plasma, and analyzed by Diffusive Reflectance Infrared Fourier Transform and Raman spectroscopy. Chemical changes of the growing films are discussed in terms of subplantation processes and interface effects. After an initial intermixing between DLC and PET forming an interlayer, the epitaxial growth of a polymer-like DLC structure is observed. For higher depositions a structural modification between the polymer-like to a more diamond-like DLC configuration is revealed. This transition is related to the folding of dehydrogenated sp2 segmented chains with subsequent rearrangement of the DLC network in higher depositions.

O 78.9 Thu 12:30 S052

Bioinspired dry adhesives from carbon nanotubes — •Christian Lutz[1], Julia Syurik[1], Sharali Malik[2], Sergei Lebedkin[2], and Hendrik Hölscher[1] — [1]Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT), 76344 Karlsruhe, Germany — [2]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

Geckos show amazing adhesive properties and are able to walk on walls and hanging on ceilings. Their adhesion force originates from nanostructures on their feet. Millions of hierarchical hairs contact the surface to generate van der Waals forces.

Mimicking the gecko structures can lead to artificial dry adhesives with a great range of applications (e.g. in robotics, medicine and space technology). While most dry adhesives are polymer-based and have benefits of easy fabrication routs and low cost production, they are not applicable at high temperatures and pressures. Carbon nanotubes (CNTs) are stable at high temperatures and, therefore, very promising as artificial adhesives for specific applications. Several scientific groups have already demonstrated dry adhesives from carbon nanotubes (CNTs). Which is due to their high aspect ratio the effective elastic modulus of the tips of CNTs is dropping below 100 kPa according to the contact splitting theory. Thus, for a free standing array of CNTs the resulting adhesive force depends on aspect ratio of CNTs and array density. In this work we analyse the relation between geometry of CNT arrays (i.e. diameter of CNTs, their height and density) and resulting pull-off force measured by AFM (force-distance curves).

O 78.10 Thu 12:45 S052

Adsorption of diclofenac on single-walled carbon nanotubes — •Mariana Kozlowska[1], Pawel Rodziewicz[1], Marta Ziegler-Borowska[2], and Anna Kaczmarek-Kedziera[2] — [1]University of Bialystok, Ciolkowskiego Str. 1K, 15-245 Bialystok, Poland — [2]Nicholas Copernicus University, Faculty of Chemistry, Gagarina 7, 87-100 Torun, Poland

Diclofenac belongs to the nonsteroidal anti-inflammatory drugs that can interact efficiently with biopolymers and carbon materials on the way of physisorption or/and chemisorption. This allows to apply carbon-based materials for the removal of diclofenac and its metabolites from water because of their hazardous impact on the environment. In order to model the efficient sorption material the systematic theoretical description of the interactions between diclofenac and carbon-based material is needed.

Therefore, we investigate the noncovalent adsorption of diclofenac on single-walled carbon nanotube (SWCNT)(10,0) using density functional theory (DFT) calculations and Car-Parrinello molecular dynamics simulations (CP-MD). We analyze the adsorption energies and the most stable adsorption patterns. Additionally, CP-MD simulations are used to mimic the properties of the dicofenac molecule adsorbed and estimate its adsorption affinity at finite temperature.

The authors gratefully acknowledge the financial support of National Science Centre, Poland, grant number 2014/13/B/ST8/04342.

O 79: Graphene III: Electronic Properties

Time: Thursday 10:30–12:45 Location: S053

O 79.1 Thu 10:30 S053

PEEM of epitaxial graphene on silicon carbide — •Richard Hönig, Christoph Keutner, Cornelis Hilscher, Ulf Berges, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

Graphene is a promising candidate for two-dimensional electronic structures. Especially epitaxial graphene on silicon carbide (SiC) is in the focus of current studies, due to the well-established infrastructure for SiC in the semiconductor-industry.

We present photoemission electron microscopy (PEEM) studies of epitaxial graphene, grown by confinement controlled sublimation (CCS). This technique is a suitable tool for producing large areas of homogeneous graphene. The resulting flake-sizes of graphene exceed the resolution of scanning tunneling microscopy. However, the PEEM-technique provides a better suited resolution up to the mesoscopic scale. Hence, PEEM was chosen to study and characterize these graphene/SiC-samples.

Here, we will demonstrate the first characterization procedures and results. In the future, samples with an adequate amount of graphene will be used for further studies, including the real-time imaging of intercalation-processes.

O 79.2 Thu 10:45 S053

Graphene growth on structured SiC — •Alexander Stöhr[1], Jens Baringhaus[2], Aleixei Zakharov[3], Christoph Tegenkamp[2], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Deutschland — [2]Leibniz-Universität Hannover, Hannover, Deutschland — [3]MAX IV Laboratory, Lund University, Lund, Schweden

Despite its missing band gap, graphene is reviewd as a potential successor of silicon for applications in logical devices. Nowadays, few techniques are available to introduce a band gap into the band structure of graphene. One of the most promising methods is the confinement of its charge carriers into quasi one-dimensional stripes, so called graphene nanoribbons. Unfortunately, the usual approach to structure graphene by lithography techniques leads to disorder and defects at the edges of the nanoribbons, which then dominat the electronic states of the ribbon. To circumvent this problem, we structure our SiC-crystal prior to the graphene growth. After the growth process a faceting of the sidewalls by 23-28° was observed by AFM. On those areas which are inclined towards the non-structured surface, diffraction spots and a π-band were observed in microscopic LEED and ARPES, respectively. Those experimental findings confirm the growth of ordered graphene on the facets.

O 79.3 Thu 11:00 S053

A new candidate for silicon carbide (3x3) surface reconstruction — •Jan Kloppenburg[1,3], Lydia Nemec[2,3], Björn Lange[4], Matthias Scheffler[3], and Volker Blum[4] — [1]Université catholique de Louvain — [2]Technische Universität München — [3]FHI Berlin — [4]Duke University

Silicon carbide (SiC) is a primary substrate for high quality epitaxial graphene growth. Graphene growth on SiC(000-1) surface is significantly different from the well controlled monolayer graphene growth on the silicon face. On the carbon face, a (3x3) surface as a precursor phase precedes graphene growth changing the thermodynamics compared to the Si-face[1]. Despite more than a decade of research the precise atomic structure of the (3x3) surface reconstruction of SiC(000-1) is still not clear. Here, we employ an *ab initio* random structure search (AIRSS) based on van-der-Waals corrected PBE density functional theory (DFT) to identify the reconstruction in the C-rich range. Our search reveals a new lowest energy surface reconstruction model for the C-rich SiC(000-1) face that was not previously reported[2] and that would explain the very different graphitization behaviour compared to the Si-face. Simulated STM images are in excellent agreement with previously reported experimental findings[3,4].

[1] Nemec et al, *Phys. Rev. Lett.* **111**, 065502, 2013
[2] Nemec et al, *Phys. Rev. B* **91**, 161408, 2015
[3] Hiebel et al, *Phys. Rev. B* **80**, 235429, 2009
[4] Hiebel et al, *Phys. Rev. B* **45**, 154003, 2011

O 79.4 Thu 11:15 S053

Characterisation of Graphene Electrodes — •Markus Manz[1], Martin Lottner[1], Martin Stutzmann[1], and Jose Garrido[1,2] — [1]Walter Schottky Institut, Technische Universität München, Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

The biocompatibility and flexibility of graphene devices allow for long-term in vivo detection of action potentials [1]. Thus, graphene has a serious advantage over former approaches [2] using other materials, which are rigid or brittle. Furthermore, the transparency of graphene micro electrodes allows for simultaneous optical stimulation/imaging and electrical recording [1]. While graphene has a high in plane conductivity, the out of plane conductivity of undoped single layer graphene (SLG) is rather low. This is a major drawback for the detection of neurotransmitters through their respective redox reactions. Therefore, various methods have been developed to increase the out of plane conductivity and 'activate' [3] the SLG electrodes. We investigated two methods of graphene 'activation', namely ozonization and doping with nitric acid. We characterized the modified electrodes using cyclic voltammetry, impedance spectroscopy, and Raman spectroscopy. We then compared the sensitivity of the untreated and 'activated' electrodes towards the neurotransmitters norepinephrine and dopamine.

[1] Kuzum, D. et al., Nat. Commun. 5:5259doi: 10.1038/ncomms6259 (2014). [2] Kwon, K. Y. et al. in Biomedical Circuits and Systems Conference (BioCAS), 2012 IEEE 164-167 (2012). [3] Kasry, A. et al., ACS Nano 4, 3839-3844 (2010).

O 79.5 Thu 11:30 S053

Ultraclean Freestanding Graphene by Pt-metal catalysis — •Jean-Nicolas Longchamp, Conrad Escher, and Hans-Werner Fink — Physics Department of the University of Zurich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

When using graphene as a substrate in electron microscopy, the presence of residues is obstructive because the latter are often of the same size as the object under study. While the growth of defect-free single-layer graphene by means of chemical vapor deposition (CVD) is nowadays a routine procedure, easily accessible and reliable techniques to transfer graphene to different substrates in a clean manner are still lacking. We have discovered a method for preparing ultraclean freestanding graphene using the catalytic properties of platinum metals. Complete catalytic removal of a sacrificial PMMA layer only requires annealing in air at a temperature between 175°C and 350°C. Here, we will describe in detail the preparation process for obtaining ultraclean freestanding graphene by Pt-metal catalysis. The presentation of low-energy electron holography and TEM investigations will demonstrate that areas of ultraclean freestanding graphene as large as 2 microns square can now routinely be prepared.

O 79.6 Thu 11:45 S053

Nano-scaled graphene solution-gated field-effect transistors — •Peter Knecht[1], Benno Martin Blaschke[1], Karolina Stoiber[1], Martin Letter[1], Simon Drieschner[1], and Jose Antonio Garrido[2] — [1]Walter Schottky Institut, TU München, Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

Graphene solution-gated field-effect transistors (SGFETs) are a promising biosensing platform, due to their unique properties such as high charge carrier mobility, low electronic noise, good electrochemical performance and an excellent biocompatibility. The recording of cell action potentials using graphene SGFETs has already been demonstrated. However, the sensing area of several hundred square micrometer is not small enough to resolve potential changes on a subcellular level. In this work, we present the fabrication of nano-scaled graphene SGFETs where the transistor area is reduced to 0.01 square micrometer. The dependence of the transistor's transconductance and the electronic low frequency noise on size and shape of the sensing area is studied. In addition, we investigate if the reduced device size leads to a more pronounced dependence of the device's performance on the graphene quality. Finally, the recording of cell action potentials using the nano-scaled devices is demonstrated and compared to micro-scaled graphene SGFETs.

O 79.7 Thu 12:00 S053

Graphene wrinkles: their conductivity, crystallinity, and reactivity — •Raul D. Rodriguez[1,2], Tao Zhang[3], Jana Kalbacova[1,2], Devang Parmar[1], Akhil Nair[1], Zoheb Khan[1], Mahfujur Rahaman[1], Ihsan Amin[2], Jacek Gasiorowski[1], Evgeniya Sheremet[1], Rainer Jordan[2], Michael Hietschold[1], and Dietrich R.T. Zahn[1,2] — [1]Institut für Physik, Technische Universität Chemnitz, Chemnitz 09107, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Germany — [3]Professur für Makromolekulare Chemie, Department Chemie, Technische Universität Dresden, Mommsenstrasse 4, 01062 Dresden, Germany

Wrinkles appear to be unavoidable in graphene produced by chemical vapor deposition (CVD) on copper. Despite its generality, isolating the role of wrinkles on overall electrical conductivity, crystallinity, and chemical reactivity of CVD-grown graphene remains an open issue. We investigate the reactivity of basal planes and wrinkles in graphene with polystyrene bromide (PSBr) and correlate it with electrical conductivity, defect concentration, and doping with a special resolution from the micro- to the nano-scale. We show that wrinkles dominate the chemical reactivity of CVD graphene, and moreover, that doping with the same functionality can yield opposite electronic type to the basal plane regions (n- vs. p-type). These results expand our understanding of wrinkles in CVD graphene towards engineering for novel applications.

O 79.8 Thu 12:15 S053

Conversion of pyrrolyl-thiophenol self-assembled monolayers (SAMs) into carbon nanomembranes (CNMs) and graphene — •Christof Neumann[1], Matthias Füser[2], Michael Mohn[3], Ute Kaiser[3], Andreas Terfort[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Institute of Inorganic and Analytical Chemistry, Goethe University Frankfurt, 60348 Frankfurt — [3]Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm

The conversion of aromatic self-assembled monolayers (SAMs) into carbon nanomembranes (CNMs) and graphene presents a promising pathway to the production of a broad variety of functional 2D materials [1]. The properties of these materials can be flexibly tuned via an appropriate choice of the molecular building units for SAMs. Here we investigate the conversion of 4-(1H-pyrrol-1-yl)thiophenol and 4-(2,5-dimethyl-1H-pyrrol-1-yl)thiophenol SAMs on polycrystalline copper foils into CNMs via the electron induced crosslinking. Furthermore, we study the pyrolytic transformation of these CNMs into graphene at temperatures up to 800 °C. We characterize these different conversion steps and the resulting physical and chemical properties of CNMs and graphene by a number of complementary experimental techniques including X-ray photoelectron and Raman spectroscopy, high-resolution transmission electron and helium ion microscopy as well as by electric transport measurements. [1] P. Angelova et al.,: A Universal Scheme to Convert Aromatic Molecular Monolayers into Functional Carbon Nanomembranes, ACS Nano 7, 6489 (2013)

O 79.9 Thu 12:30 S053

Extracellular stimulation of electrogenic cells using graphene devices — •Karolina Stoiber[1], Martin Lottner[1], Markus Manz[1], Simon Drieschner[1], Benno Blaschke[1], Martin Stutzmann[1], and José A. Garrido[1,2] — [1]Walter Schottky Institut, Technische Universität München, Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

Graphene is a highly conductive, chemically stable, flexible and biocompatible material. Therefore, Graphene microelectrode arrays (GMEAs) are a promising bio-sensing and cell stimulation platform in neural implants. In this work, the electrical stimulation of HEK293 and HL1 cells through extracellular voltage trains by GMEAs is presented. Further, the investigation of the biocompatibility of graphene foam and its capability for extracellular stimulation is discussed.

GMEAs with circular electrodes were fabricated using standard photo-lithography techniques. For the characterization of the devices Raman-spectroscopy and cyclic voltammetry were used. The cell membrane potential of HEK293 cells was monitored during extracellular stimulation via patch-clamping. HL1 cells, a cardiomyocyte-like cell line, were dyed with a calcium-sensitive fluorophore and the modulation of their firing frequency upon stimulation was recorded.

Graphene foam devices were fabricated as previously described. The devices were characterized electrochemically and their capability for extracellular stimulation of HL1 cells tested.

O 80: Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV

Time: Thursday 10:30–13:15 Location: H24

Topical Talk O 80.1 Thu 10:30 H24

Transport phenomena in broken-symmetry metals: Geometry, topology, and beyond — •Ivo Souza — Universidad del País Vasco, San Sebastián, Spain

While topological quantization is usually associated with gapped systems – Chern insulators and topological insulators – it can also occur in broken-symmetry metals, where the Fermi surface (FS) consists of disjoint sheets: the Berry-curvature flux through each sheet is quantized, defining an integer Chern index. Using ferromagnetic bcc Fe as an example, I will describe how the FS Chern numbers are related to the chiral degeneracies ("Weyl points") in the bandstructure. When placed in a static magnetic field, a Weyl (semi)metal will display the chiral magnetic effect (CME), where an electric field pulse $\mathbf{E} \parallel \mathbf{B}$ drives a transient current $\mathbf{j} \parallel \mathbf{B}$. Weyl semimetals with broken inversion and mirror symmetries can also display a "gyrotropic magnetic effect" (GME), where an oscillating magnetic field drives a current and, conversely, an electric field induces a magnetization. The GME is the low-frequency limit of natural optical activity. It is governed by the intrinsic magnetic moment (orbital plus spin) of the Bloch electron on the FS, in much the same way that the anomalous Hall effect and CME are governed by the FS Berry curvature. Like the Berry curvature, the intrinsic magnetic moment should be regarded as a basic ingredient in the Fermi-liquid description of transport in broken symmetry metals.

Topical Talk O 80.2 Thu 11:00 H24

Dirac Fermions in Antiferromagnetic Semimetal — •Peizhe Tang, Quan Zhou, Gang Xu, and Shou-Cheng Zhang — Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA

The analogues of elementary particles in condensed matter systems have been extensively searched for because of both scientific interests and technological applications. Recently massless Dirac fermions are found to emerge as low energy excitations in the materials named Dirac semimetals. The currently known Dirac semimetals are all nonmagnetic with both time-reversal symmetry T and inversion symmetry P. Here we show that Dirac fermions can exist in one type of antiferromagnetic systems, where T and P are broken but their combination PT is respected. We propose orthorhombic antiferromagnet CuMnAs as a candidate, analyze the robustness of the Dirac points with symmetry protections, and demonstrate its distinctive bulk dispersions as well as the corresponding surface states by ab initio calculations. Our results give a new routine towards the realization of Dirac materials, and provide a possible platform to study the interplay of Dirac-related physics and magnetism.

O 80.3 Thu 11:30 H24

Spin Hall effect in non-collinear antiferromagnets Mn3X (X=Sn, Ge, Ga) — •Yang Zhang[1,3], Yan Sun[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany

Recently, large anomalous Hall effect (AHE) was realized in non-collinear antiferromagnetic (AFM) compounds Mn3X (X=Sn, Ge, Ga). We have found that the nonzero Berry curvature – origin of the AHE observed – will lead to another topological effect, the spin Hall effect (SHE) in the titled compounds. We have systematically investigated the intrinsic SHE and revealed large spin Hall conductivity [˜1000 ((*/e)*(S/cm)], which is comparable to that of the well-know SHE material Pt. Our work present a new family of AFM compounds for the room-temperature spintronic applications.

O 80.4 Thu 11:45 H24

Electronic reconstruction and anomalous Hall conductivity in $3d$-oxide honeycomb lattices within the corundum structure — •santu baidya and rossitza pentcheva — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg

The electronic structure of $3d$ transition metal oxide honeycomb layers confined in the corundum structure (α-Al$_2$O$_3$) along the [0001] direction is investigated using density functional theory including an on-site Coulomb term (GGA+U). While in some cases (e.g. $(M_2\mathrm{O}_3)/(\mathrm{Al}_2\mathrm{O}_3)_5$, M=Fe, Co, V, Cr, Ni) the confined geometry preserves the magnetic and electronic ground state properties of the corresponding bulk corundum compound $M_2\mathrm{O}_3$, strong deviations from the bulk behavior are observed in the case of Ti$_2$O$_3$ and Mn$_2$O$_3$ bilayers. Our results indicate a formation of a quasi two-dimensional electron gas with a vertical confinement of ∼5 Å for Ti$_2$O$_3$ and ∼8.5 Å for Mn$_2$O$_3$. As a function of lateral strain (Ti$_2$O$_3$)/(Al$_2$O$_3$)$_5$ undergoes a metal-to-insulator transition associated with a switching of orbital polarization. In the metallic state the Dirac point can be tuned to the Fermi level by variation of the c/a ratio. Including spin-orbit coupling a finite anomalous Hall conductivity is observed in $(M_2\mathrm{O}_3)/(\mathrm{Al}_2\mathrm{O}_3)_5$ (M=Ti, Mn).

O 80.5 Thu 12:00 H24

Anomalous hall effect in triangular antiferromagnetic ordered structure — •Hao Yang[1], Sun Yan[2], Felser Claudia[2], Parkin Stuart[1], and Binghai Yan[2] — [1]Max Planck Institute of Microstructure Physics, 06120 Halle(Saale), Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The anomalous Hall effect (AHE), a fundamental transport phenomenon of electrons in solids, has been believed to appear in ferromagnetic materials. Very recently AHE is revealed in noncollinear antiferromagnetic compounds. In this work, we have systematically investigated the AHE in antiferromagnetic materials Mn3X (X=Ir, Ge, Sn, Ga), where noncollinear 120-degree type antiferromagnetic spin order exists in the quasi-layered lattice. Assisted by the symmetry analysis, we demonstrate the strong anisotropy of the intrinsic anomalous Hall conductivity that is determined by the Berry curvature in the band structure. Our work well interprets recent experiment observations and predicts novel antiferromagnetic material candidates for the spintronic application.

O 80.6 Thu 12:15 H24

Anomalous Hall conductivity and orbital magnetization as local quantities — •Antimo Marrazzo[1] and Raffaele Resta[2] — [1]THEOS, EPF Lausanne, Switzerland — [2]Dipartimento di Fisica, Univ. Trieste, Italy

Anomalous Hall conductivity (AHC) and orbital magnetization (OM) are—from a theorist's viewpoint—closely related: both have an expression as **k**-space integrals of the appropriate geometrical quantity. The **k** space is an artificial construct: all bulk properties are embedded in the ground state density matrix in **r** space, independently of the boundary conditions. Is it possible to address AHC and OM as local properties, directly in **r** space? For insulators, two recent papers have proved that the answer is affirmative: both AHC (quantized in insulators) and OM can be evaluated from a local formula over bounded samples. A rationale can be found in the "nearsightedness" of the density matrix: but since this is *qualitatively* different in insulators and metals (exponential vs. power law) it is not obvious that the same successful approach can be extended to metals. Using model Hamiltonians, we have performed simulations over 2D bounded metallic flakes, where the T-invariance is broken in two alternative ways: either à la Haldane, or by a macroscopic **B** field. In both cases, our simulations show that the relevant quantity can be extracted from a knowledge of the electron distribution in the bulk region of the sample only. This looks counterintuitive because the OM of a magnetized sample owes to currents localized near its surface; but the key reason for the success of the local approach to AHC and OM is that the formulas are *not* based on currents.

O 80.7 Thu 12:30 H24

Laser induced DC photocurrents in a Topological Insulator thin film — •Thomas Schumann[1], Nina Meyer[1], Gregor Mussler[4], Eva Schmoranzerová[2], Dagmar Butkovicova[2], Helena Reichlová[3], Lukas Braun[5], Christian Franz[6], Michael Czerner[6], Pertr Němec[2], Detlev Grützmacher[4], Tobias Kampfrath[5], Christian Heiliger[6], and Markus Münzenberg[1] — [1]IfP, EMA University Greifswald, Germany — [2]MFF, Charles University, Prague, Czech Republic — [3]FZU, Prague, Czech Republic — [4]PGI-9, Jülich, Germany — [5]FHI Berlin, Germany — [6]University of Gießen, Germany

Topological Insulators (TI) open up a new route to influence the transport of charge and spin in a surface film via spin-momentum locking [1,2]. It has been demonstrated experimentally [2] that illumination by circularly polarized light can result in excitation of a helicity-dependent photocurrent.We report our recent results on laser induced photocurrents in a terniary 3D TI thin film. The resulting photocurrents are classified after [1,2] and we show that there are at least two signals visible, for example in time dynamics, which behave different in the suggested parameters.

We acknowledge the funding of the DFG via the SPP 1666 Topological Insulators and the joint DAAD PPP Czech Republic project FemtomagTopo. [1]S.D.Ganichev,W.Prettl,J.Phys.: Condens. Matter 15 (2003) R935-R983

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O 80.8 Thu 12:45 H24

Robustness of exchange protocols of Majorana fermions in quantum wire networks — •Christian Tutschku[1], Rolf W. Reinthaler[1], Chao Lei[2], Allan H. MacDonald[2], and Ewelina M. Hankiewicz[1] — [1]Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Department of Physics, University of Texas at Austin, USA

The interface between topological non-trivial, one-dimensional, spinless p-wave superconductors and the vacuum is connected to the appearance of Majorana edge-modes [1], whose non-trivial exchange statistics makes them promising candidates for topological quantum computation [2]. Via T-Bar structures build of 1D-nanowires we can manipulate and exchange the Majorana fermions by purely electrical means [3]. By applying a tight binding approach we solve the time dependent Bogoliubov-de Gennes equations for the Kitaev chain model [1] and also cure the problem of an appearing additional Majorana-boundstate located at the T-Bar crossing point for small lattice constants. Furthermore we analyze how the robustness of the exchange protocols is affected by non-adiabatic effects or by a finite overlap of the Majorana bound states.

We acknowledge financial support by the DFG within SFB 1170 ToCoTronics.

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[3] J. Alicea et al., Nature Physics **7**, 412 (2011)

O 80.9 Thu 13:00 H24

Unpaired Majorana modes in Josephson junctions arrays with gapless bulk excitations — •Manuel Pino Garcia — Department of Physics and Astronomy, Rutgers The State University of New Jersey, 136 Frelinghuysen rd, Piscataway, 08854 New Jersey, USA

The search for Majorana bound states in solid-state physics has been limited to materials which display a gap in their bulk spectrum. We will show that such unpaired states appear in certain quasi-one-dimensional Josephson junctions arrays with gapless bulk excitations. The bulk modes mediate a coupling between Majorana bound states via the Ruderman-Kittel-Yosida-Kasuya mechanism. As a consequence, the lowest energy doublet acquires a finite energy difference. For realistic set of parameters this energy splitting remains much smaller than the energy of the bulk eigenstates even for short chains of length L ~ 10. In this talk, we first explain the JJA system and how to model it with an Ising-like Hamiltonian. Then, a qualitative argument is employed to obtain the low-energy effective theory using unpaired Majorana modes. We will show numerical results which confirm the validity of this effective theory and discuss problems that may arise in the experimental realization of our proposal.

O 81: Oxides and Insulator Surfaces I

Time: Thursday 10:30–13:30 Location: H4

Invited Talk O 81.1 Thu 10:30 H4

Imaging orbitals and defects in superconducting FeSe/SrTiO$_3$ — •Jennifer Hoffman[1,2], Dennis Huang[1], Tatiana Webb[1], Shiang Feng[1], Can-Li Song[1,3], Cui-Zu Chang[4], Jagadeesh Moodera[4], and Efthimios Kaxiras[1] — [1]Harvard University, Cambridge, MA, USA — [2]University of British Columbia, Vancouver, Canada — [3]Tsinghua University, Beijing, China — [4]Massachusetts Institute of Technology, Cambridge, MA, USA

Single-layer FeSe grown epitaxially on SrTiO$_3$ has been shown to superconduct with T_c as high as 100 K, more than a factor of 10 higher than bulk FeSe. This dramatic enhancement motivates intense efforts to understand the superconducting mechanism and to design and fabricate devices. Nematic order, breaking the 4-fold rotational symmetry of the crystal, has been proposed as an important factor in the superconducting phase diagram. Meanwhile, atomic defects, which may pin nematic fluctuations or otherwise perturb superconductivity, can provide important clues into the superconducting mechanism as well as practical routes to superconducting devices. Here we use scanning tunneling microscopy (STM) to search for orbital nematicity in single-layer FeSe/SrTiO$_3$, and to investigate atomic-scale defects which locally influence superconductivity. From quasiparticle interference (QPI) images, we disentangle scattering intensities from the orthogonal Fe $3d_{xz}$ and $3d_{yz}$ bands, and quantitatively exclude pinned nematic orbital order with domain size larger than $\delta r \sim 20\,\mathrm{nm}$. Furthermore, we identify a prevalent "dumbbell"-shaped atomic-scale defect whose placement could be harnessed to define two-dimensional superconducting devices.

O 81.2 Thu 11:00 H4

Surface structure of Fe$_3$O$_4$(110) investigated by Scanning Tunneling Microscopy and Density Functional Theory. — •Brian Walls, Olaf Lübben, and Igor V. Shvets — School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland

We have performed a combined Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT) study of the (110) surface of single crystalline magnetite (Fe$_3$O$_4$). The (110)-terminated surface consists of two alternating planes, namely the A and B planes. Previous STM studies of the Fe$_3$O$_4$(110) surface have shown an A-plane terminated row reconstruction [1,2]. However, in this work STM measurements reveal not just the row reconstruction, but also an atomically flat surface structure which is present when the rows break. Interestingly, this flat structure lies just ~3Å below the adjacent rows.

DFT calculations were performed in order to gain an understanding of the flat structure. The calculations indicate that the presence of vacancies leads to an energetically favourable model and a good match between simulated STM images (Tersoff-Hamann scheme) and experimental images.

References:

1. R. Jansen *et al.*, *Surf. Sci.* **328**, 237-247 (1995).
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O 81.3 Thu 11:15 H4

Simulating atomic-scale phenomena on surfaces of unconventional superconductors — •Andreas Kreisel[1], Peayush Choubey[2], Tom Berlijn[3], Brian Andersen[1], and Peter Hirschfeld[2] — [1]Niels Bohr Institute, Denmark — [2]Univ. of Florida, USA — [3]CNMS & CSMD, Oak Ridge Nat. Lab., USA

Interest in atomic scale effects in superconductors has increased because of two general developments: First, the discovery of new materials as the cuprate superconductors, heavy fermion and Fe-based superconductors where the coherence length of the cooper pairs is as small to be comparable to the lattice constant, rendering small scale effects important. Second, the experimental ability to image sub-atomic features using scanning-tunneling microscopy which allows to unravel numerous physical properties of the homogeneous system such as the quasi particle excitation spectra or various types of competing order as well as properties of local disorder. On the theoretical side, the available methods are based on lattice models restricting the spatial resolution of such calculations. In the present project we combine lattice calculations using the Bogoliubov-de Gennes equations describing the superconductor with wave function information containing sub-atomic resolution obtained from *ab initio* approaches. This allows us to calculate phenomena on surfaces of superconductors as directly measured in scanning tunneling experiments and therefore opens the possibility to identify underlying properties of these materials and explain observed features of disorder. It will be shown how this method applies to the cuprate material Bi$_2$Sr$_2$CaCu$_2$O$_8$ and a Fe based superconductor.

O 81.4 Thu 11:30 H4

Decomposition of the model perovskite SrTiO$_3$ under electrochemical stress — •Christian Rodenbücher, Gustav Bihlmayer, Paul Meuffels, Rainer Waser, and Kristof Szot — Peter-Grünberg-Institut, Forschungszentrum Jülich, 52425 Jülich

Transition metal oxides are the key materials for future energy-efficient electronics in particular for logic and memory devices based on the resistive switching effect. Since the switching effect is related to a local reaction of the oxide to an external gradient of the electrical and chemical potential, we investigate the influence of electrochemical stress on the prototype perovskite SrTiO$_3$. We demonstrate that upon application of a DC voltage under UHV conditions, the surface region of alkaline earth titanates transforms into lower binary oxides with nanoporous structure. By means of IRT, XPS, EDX, HR-TEM, and LC-AFM we present that this transformation takes place at relatively low temperatures and is related to a fundamental macroscopic decomposition of the oxide changing the physical properties of the surface region up to depths of several tens of micrometers. Our results demonstrate that in ternary oxides phase transformations can be induced by gradients of the electrochemical potential using a technologically simple method, which not only opens up a new way for tailoring micro layers of functional transition metal oxides with bespoke properties for optical, electronic and chemical applications but also demonstrates the mutability of metal oxides under electrical stress being relevant for the understanding of the electroforming and switching process in novel memristive devices.

O 81.5 Thu 11:45 H4

Electronic structure of $CeTiO_4$ — •Lukas Sojka[1] and Dominik Legut[2] — [1]FMMI, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

Cerium titanate structures offer broad range of technological applications because of their optical and catalytic properties. Cerium titanate can form various phases, which depend on the oxidation state of cerium. Using the first-principle calculations, we identified the ground-state structure of a new found phase, $CeTiO_4$. In analogy with $LaTaO_4$, the calculated enthalphy of formation indicates that the most stable structure is the monoclinic one over the orthorhombic structure, and its stability is by factor four higher than in $LaTaO_4$. Based on the calculated electronic structure we determined optical properties, mechanical properties (elastic constants) and thermodynamical properties of both structures of $CeTiO_4$. The results were obtained using single-electron framework of density functional theory calculations employing the VASP code. our results also indicate that cerium is in the oxidation state of Ce^{4+}.

O 81.6 Thu 12:00 H4

DFT calculations of the electronic and atomic structure of metal-oxide nanowires formed on Ir(100) — Florian Mittendorfer[1], Pascal Ferstl[2], Matthias Gubo[2], Klaus Heinz[2], M.Alexander Schneider[2], Lutz Hammer[2], and •Josef Redinger[1] — [1]Inst. of Applied Physics, TU Wien, Vienna, Austria — [2]Lehrstuhl für Festkörperphysik, Univ. Erlangen-Nürnberg, Erlangen, Germany

Recently, a self-organized growth of quasi one-dimensional ordered cobalt oxide nanowires on the Ir(100) surface has been witnessed. By deposition of 1/3 ML Co in oxygen rich conditions nanowires of either CoO$_2$ or CoO$_3$ stoichiometry are formed, which bind via oxygen to the Ir substrate and leave the Co chains almost completely decoupled from the substrate. We report on DFT calculations for nanowires of CoO$_2$ and CoO$_3$ type as well as their Ni, Fe and Mn analogues. We find a very good agreement with experimental data concerning structural details and predict an electronic structure which is not strictly one-dimensional, despite the structural decoupling of the metal atoms from the substrate. First results of collinear calculations indicate a change of magnetism proceeding from nonmagnetic NiO_2, via ferromagnetic CoO_2 and FeO_2 to antiferromagnetic MnO_2.

O 81.7 Thu 12:15 H4

Two-Dimensional Iron Tungstate Honeycomb Layers on Pt(111) — •Sascha Pomp[1], David Kuhness[1], Giovanni Barcaro[2], Luca Sementa[2], Alessandro Fortunelli[2], Martin Sterrer[1], Falko P. Netzer[1], and Svetlozar Surnev[1] — [1]Institute of Physics, University of Graz, A-8010 Graz, Austria — [2]CNR-ICCOM & IPCF, Consiglio Nazionale delle Ricerche, I-56124 Pisa, Italy

We report the first example of a 2D ternary oxide layer with a honeycomb geometry identified as FeWO3, which has no bulk analogue. The 2D iron tungstate phase described here has been synthesized in UHV via a solid state reaction of (WO3)3 clusters with a FeO monolayer on a Pt(111) surface. It has been characterized by a variety of surface analytic techniques, involving x-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM), low-energy electron diffraction (LEED) and temperature programmed desorption (TPD), combined with density functional theory (DFT) calculations. Consistent with the experimental results, the DFT calculations show that the FeWO3 layer consists of a mixed layer of Fe and W atoms, formally Fe2+ and W4+ species, sitting in fcc and hcp Pt hollow sites, respectively, and arranged in a (2x2) superstructure. This layer is terminated by oxygen atoms in Fe-W bridging positions, forming a buckled honeycomb lattice. In addition the DFT calculations predict that the 2D FeWO3 layer exhibits ferromagnetic order with a Curie temperature of 95 K, as opposed to the antiferromagnetic behavior in the bulk FeWO4 phase.

O 81.8 Thu 12:30 H4

In-situ electron microscopy studies of praseodymia on Ru(0001) — •Jon-Olaf Krisponeit[1], Jan Höcker[1], Andreas Schäfer[2], Julian Cambeis[1], Alexei Zakharov[2], Yuran Niu[2], Jens Falta[1], and Jan Ingo Flege[1] — [1]University of Bremen, Bremen, Germany — [2]Lund University, Lund, Sweden

Due to the multiple valence states of rare earth elements, their oxides (REOs) play an important role in catalysis applications. A prominent example is ceria, which is well known for its oxygen storage capacity. Grown as microparticles on Ru(0001), ceria shows an excellent crystalline quality and thermal stability, making it well suited for catalytic model studies. We extend these efforts to the less studied praseodymia, which exhibits an intriguingly complex phase diagram with many stable mixed-valence compounds between Pr_2O_3 and the fully-oxidized PrO_2. Furthermore, praseodymia shows the highest oxygen mobility among the REOs, rendering PrO_x/Ru(0001) an attractive inverse catalyst model system.

We have prepared ultra-thin films of PrO_x/Ru(0001) by reactive molecular beam epitaxy. Here, we present in-situ investigations on local morphology and structure by low energy electron microscopy and micro-illumination diffraction (LEEM/μ-LEED), revealing the nucleation of triangular islands and the formation of rotational domains. Furthermore, we studied the local chemical composition by x-ray absorption spectroscopy in imaging mode (XAS-PEEM) and discuss post-oxidation and reduction processes as identified by x-ray photoelectron spectroscopy (XPS).

O 81.9 Thu 12:45 H4

Electronic structure of ultra-thin ZnO on Metal substrates — •Bjoern Bieniek[1], Patrick Rinke[2], Oliver T. Hofmann[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Aalto University, Helsinki, Finland — [3]TU Graz, Austria

ZnO is a promising candidate for applications in opto-electronics. For a successful application stable n-type and p-type ZnO would be needed. As for many wide band gap semi-conductors, p-type conductivity is difficult to achieve in ZnO. We propose ZnO ultra-thin films on metal substrates as model systems for investigating p-type conductivity in ZnO. In our investigation of the electronic structure of ultra-thin ZnO films (1 to 4 layers) on the (111) surfaces of Ag, Cu, Pd, Pt, Ni, and Rh by means of DFT with the PBE and HSE06 exchange-correlation functionals we find a novel mechanism to achieve p-type conductivity at the surfaces of ZnO thin films on metal substrates. This mechanism is based on the intrinsic polar nature of ZnO $(000\bar{1})$ films. With increasing thickness the polar character of wurtzite ZnO emerges as the films structurally transform from α-BN to wurtzite. electrons are transferred from the Zn-terminated interface to adjacent layers. The resulting field shifts the electronic states upwards until the Fermi energy, provided by the metal, is reached and the film becomes effectively p-type doped at its surface by pinning the electronic states of the top most layer(s) at the Fermi level. The number of layers necessary to achieve effective p-type doping depends on the metallic substrate. We also discuss intrinsic defects in the ZnO films on metal substrates.

O 81.10 Thu 13:00 H4

Role of dopants on the performance of metal oxide surfaces for the water oxidation:a DFT+U approach — •hamidreza hajiyani and rossitza pentcheva — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057, Duisburg

Based on density functional theory calculations including an on-site Coulomb repulsion term, we explore the oxygen evolution reaction (OER) at transition metal oxide surfaces. We address strategies how to reduce the overpotential during OER as well as modification of the band edge positions through dopants. A systematic variation of dopands throughout the $3d$, $4d$ and $5d$ series in α-Fe_2O_3 (0001) surface unravels trends concerning the role of d-band occupation and orbital polarization. Consistent with previous results, the overpotentials correlate with the binding energy of chemisorbed species within a volcano plot. The underlying mechanisms are discussed by monitoring changes of valence and spin state of the surface cations throughout the intermediate steps of OER. We further generalize our results to other oxide structures such as the spinel. Support by the DFG within priority program SPP1613, project PE883/9-2 and a computational grant at the Leibniz Rechenzentrum are gratefully acknowledged.

O 81.11 Thu 13:15 H4

DFT study of metallic adsorbates on bulk and thin films of Zirconia — •Wernfried Mayr-Schmölzer, Florian Mittendorfer, and Josef Redinger — Inst. of Applied Physics, TU Wien, Vienna, Austria

Zirconia (ZrO_2) is a material with many interesting properties, making it useful for various technological applications, such as a solid electrolyte in solid-oxide fuel-cells or as an oxygen gas sensor. Therefore, a detailed understanding of adsorption and interface properties of Zirconia is very useful. We present results of DFT calculations for the adsorption of metal adatoms and clusters on bulk surfaces and on thin Zirconia films grown by oxidation of a Pt_3Zr substrate. The calculations were performed using the Vienna Ab-Initio Simulation Package (VASP) employing van-der-Waals density functionals. The bonding and adsorption mechanism was studied for various metal adatoms such as noble Au and Ag as well as reactive Ni and Pd. On bulk surfaces we only find a weak physisorption for noble Au and even weaker for Ag ($\approx$ 0.5eV), while reactive Ni and Pd show significantly higher adsorption energies ($>$ 2.0 eV). On a thin supported ZrO_2 film a general increase of the adsorption energies by more than 0.5 eV is predicted, resulting a chemisorbed state for Ag, wheres Au remains more weakly bound. To investigate mobility and cluster formation of these noble adsorbates we report on the surface diffusion barriers for silver and gold where we find values below 0.5 eV. We also report on the interface energy of silver and gold films of varying thickness on the thin oxide film.

O 82: Structure of Solid/Liquid Interfaces I

Time: Thursday 10:30–13:00 Location: H6

O 82.1 Thu 10:30 H6

Probing the TiO_2/Liquid Interface of a Photoelectrochemical Cell by X-Ray Photoelectron Spectroscopy — •Michael F. Lichterman[1,2], Matthias H. Richter[1,2,7], Shu Hu[1,2], Ethan J. Crumlin[3], Stephanus Axnanda[3], Marco Favaro[3,4], Walter Drisdell[3,4], Zahid Hussain[3], Bruce S. Brunschwig[1], Zhi Liu[3,5,6], Nathan S. Lewis[1,2], and Hans-Joachim Lewerenz[1,2] — [1]Caltech, Pasadena, USA. — [2]JCAP, Pasadena, USA. — [3]LBNL, Berkeley, USA. — [4]JCAP, Berkeley, USA. — [5]Chinese Academy of Sciences, China. — [6]ShanghaiTech University, China. — [7]BTU C-S, Cottbus, Germany.

Amorphous TiO_2 coatings can stabilize semiconductor photoanodes such as Si, GaAs, and GaP that are otherwise unstable in aqueous media [1]. Using tender X-rays with their substantially increased inelastic mean free scattering length of photoelectrons and using the classical three-electrode potentiostatic arrangement allows one to follow of the influence of the applied potentials on the semiconductor electrode energetics such as band bending and band edge shifts directly [2, 3]. The observed shifts in binding energy with respect to the applied potential have directly revealed rectifying junction behavior on semiconducting samples. Accumulation, depletion and Fermi level pinning were observed. Additionally, the non-linear response of the core level binding energies to changes in the applied electrode potential has revealed the influence of defect-derived electronic states on the Galvani potential across the complete cell. [1] Science 344 (2014) 1005; [2] Sci Rep 5 (2015) 9788; [3] Ener & Env Sci 8 (2015) 2409

O 82.2 Thu 10:45 H6

An Electrochemical, resonant Photoemission and Ambient Pressure-X-ray Photoelectron Spectroscopic Investigation of Si/TiO_2/Ni/Electrolyte Interfaces — •Matthias H. Richter[1,2,7], Michael F. Lichterman[1,2], Shu Hu[1,2], Ethan J. Crumlin[3], Stephanus Axnanda[3], Marco Favaro[3,4], Walter Drisdell[3,4], Zahid Hussain[3], Bruce S. Brunschwig[1], Zhi Liu[3,5,6], Nathan S. Lewis[1,2], and Hans-Joachim Lewerenz[1,2] — [1]Caltech, Pasadena, USA. — [2]Joint Center for Artificial Photosynthesis, Pasadena, USA. — [3]Lawrence Berkeley National Laboratory, Berkeley, USA. — [4]Joint Center for Artificial Photosynthesis, Berkeley, USA. — [5]Chinese Academy of Sciences, China. — [6]ShanghaiTech University, China. — [7]BTU C-S, Cottbus, Germany.

Photoelectrochemical cells based on semiconductor-liquid interfaces provide a method of converting solar energy to electricity or fuels. Recently, we have demonstrated operational systems that involved stabilized semiconductor-liquid junctions [1]. The electrical and spectroscopic properties of the TiO_2/Ni protection layer system have been investigated in contact with electrolyte solutions [2, 3, 4]. From the response of the photoelectron binding energies to variations in applied potential the energetics of the solid/electrolyte interface are elucidated. The degree of conductivity depended on the chemical state of the Ni on the TiO_2 surface. The combinations of these techniques provide a powerful tool for the investigation of hybrid electrode/solution contacts. [1] Science 344 (2014) 1005; [2] Sci Rep 5 (2015) 9788; [3] Ener & Env Sci 8 (2015) 2409; [4] J Electrochem Soc 162 (2016) H1

O 82.3 Thu 11:00 H6

Model free method to measure the surface potential of colloidal particles in aqueous solution — •Grazia Gonella[1], Cornelis Lütgebaucks[2], and Sylvie Roke[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Laboratory for fundamental BioPhotonics (LBP), Institute of Bioengineering (IBI), and Institute of Materials Science (IMX), School of Engineering (STI), and Lausanne Centre for Ultrafast Science (LACUS), École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Retrieval of information regarding properties of, and processes at, interfaces is notoriously difficult especially at the surface of colloidal particles in solution. Determination of the surface potential, Φ_0, is a particularly important albeit difficult task. For instance Φ_0 affects the stability of a colloidal suspension and in turn is affected by the opening of ion-channels in a membrane, just to cite two core problems in colloids and soft matter. Computations have shown that in theory the SH scattering pattern contains enough information to determine Φ_0 without making any assumptions on the structure or state of the interface. We implement this theory and extend it to low ionic strengths and use it to determine the surface potential of a variety of colloidal systems in aqueous solution.

O 82.4 Thu 11:15 H6

Adsorption of Organic Molecules on Iron Oxide Model Surfaces in Solution — •Peter Seidel[1,2] and Martin Sterrer[1,2] — [1]Institute für Physik, Unversität Graz, Universitätsplatz 5, 8010 Graz, Österreich — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Deutschland

Single-crystalline oxide thin films supported by metals are a well-accepted class of model system for studying fundamental aspects of oxide surface and thin oxide layer chemistry and physics. In the present contribution, we report on our efforts to expand this model approach to electrochemical studies on well-ordered oxide surfaces. Single-crystalline FeO(111) and Fe3O4(111) films were grown under ultrahigh vacuum (UHV) conditions on a Pt(111) substrate and subsequently transferred into air or brought into contact with aqueous solutions. We have tested the stability of the oxide layers in these environments and characterized their electrochemical properties by cyclic voltammetry. Two different organic compunds (Catechol and Aminophthalic acid) were deposited from solution and investigated by electrochemical and UHV methods. Finally, the surface morphology and potential-dependent surface structure changes were investigated in-situ by electrochemical scanning tunneling microscopy.

O 82.5 Thu 11:30 H6

Quantitative Measurements of Electrochemical Strain using Atomic Force Microscopy — •Valon Lushta[1,2], Thomas Göddenhenrich[1], Bernhard Roling[2], and André Schirmeisen[1] — [1]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392 Gießen — [2]Physikalische Chemie,Philipps-MarburgUniversität Marburg, D-35032 Marburg

Electrochemical Strain Microscopy (ESM) has emerged as a powerful tool for probing ionic transport in battery cathode. A biased AFM tip concentrates an electric field in a nanometer-scale volume of the sample, inducing ionic intercalation or deintercalation. The intrinsic link between concentration of ionic species and the molar volume of the material results in electrochemical strain and surface displacement. The magnitude of this displacement is lower than the sensitivity of modern AFMs. The excitation signal at the tip is chosen at contact resonance frequency in order to amplify the displacement by the Q factor of the AFM cantilever. The ongoing challenges in ESM are the quantitative measurement of the displacement and understanding delocalized electrostatic forces effecting the cantilever motion. Both challenges are linked to the uncertainty of contact resonance dynamics. We demonstrate a technique to quantify the displacement and estimate the electrostatic contribution without loss of resonance amplification.

O 82.6 Thu 11:45 H6

Solvent- and deposition temperature-dependent 2D supramolecular assemblies of trimesic acid at the liquid-graphite interface revealed by scanning tunneling microscopy — •Yen D.C Nguyen, Lars Smykalla, Ha N.T Nguyen, and Michael Hietschold — TU-Chemnitz, Institute of Physics, D-09107 Chemnitz, Germany

By using scanning tunneling microscopy (STM), the polymorphism of self-assembly of trimesic acid molecules at the liquid-solid interface to graphite was investigated for different kind of solvents and temperatures of the pre-heated during deposited substrate. TMA was dissolved in phenyloctane, octanoic acid and undecanol, which have different polarity. At elevated substrate temperatures, various periodic assemblies of TMA can be obtained. By increasing the temperature of the preheated substrate, the specific 2D supramolecular network structure and the corresponding packing density can be precisely tuned in each kind of the solvents studied. The results found by STM are explained by the increased concentration of the solution at the pre-heated substrate as well as the higher mobility of the solute molecules enforcing the interactions between the molecules, in particular different hydrogen bonding motifs. Our interpretation is supported by optimizing each structure and comparing their total interactions energy calculated by PM6-DH+.

O 82.7 Thu 12:00 H6

Self-assembly of 2,2'-spirobi[4H-1,3,2-benzodioxasiline] at the solid-liquid interface controlled by solvent polarity — •Thi Ngoc Ha Nguyen[1], Doan Chau Yen Nguyen[1], Thomas Ebert[2], Stefan Spange[2], and Michael Hietschold[1] — [1]Professur Analytik an Festkörperoberflächen, Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany — [2]Professur Polymerchemie, Institut für Chemie, Technische Universität Chemnitz, Chemnitz, Germany

Self-assembled molecular architectures at solid-liquid interfaces are mainly governed by the chemical nature of solute, solvent as well as the substrate properties. When molecules solved in a solution are adsorbed at a liquid-solid interface, in addition to molecule-molecule and molecule-substrate interactions, the solvent itself can also play an important role in the formation of self-assembled monolayers. In this paper, the influence of solvent polarity on self-assembly of the 2,2'-spirobi[4H-1,3,2-benzodioxasiline][1] is investigated. Such spiro molecules are useful monomers for the so-called twin polymerization. Spiro molecules consist of two different parts, - organic and inorganic - linked together by Si-O units, which can be cleaved under the same conditions but at different rates resulting in organic and inorganic precursors for the formation of two different kinds of polymers. In this way, there are created two different types of polymers out of one kind of monomer which are interlinked together on the nanoscale creating a real nanocomposite material. The self-assembly at the liquid-solid interface of these spiro molecules reveals different adsorbate patterns driven by solvent polarity.

O 82.8 Thu 12:15 H6

Porphyrin Metalation at the Solid-Liquid Interface — •Matthias Franke[1], Florencia Marchini[2], Hans-Peter Steinrück[1], Ole Lytken[1], and Federico José Williams[2] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Germany — [2]Departamento de Química Inorganica, Analítica y Química Física, Universidad de Buenos Aires, Argentina

Porphyrins are large organic molecules with potential in numerous technical applications. Especially metalloporphyrins are promising, since the metal center coordinated to the central cavity strongly influences the functionality of these molecules. So far, on-surface metalloporphyrin synthesis in ultrahigh vacuum has been achieved by codeposition of metal atoms and subsequent annealing. However, the common way to metalate porphyrins in liquid medium is through deprotonation and coordination of a dissolved metal ion. We have transferred the liquid phase synthesis approach to the surface by metalating a free-base porphyrin (2HTPP), adsorbed on an Au(111) single crystal, by exposure to aqueous zinc acetate solution, yielding ZnTPP.[1] This reaction happens at room temperature, in contrast to the higher temperatures required for metalation by codeposited metal atoms. Metalation was followed spectroscopically by means of X-ray photoelectron spectroscopy (XPS). The project is supported by the DFG through FOR 1878 (funCOS) and by the DAAD.

[1] Franke, M.; Florencia, M.; Steinrück, H.-P.; Lytken, O.; Williams, F.; J. Phys. Chem. Lett. 2015, accepted, DOI: 10.1021/acs.jpclett.5b02218

O 82.9 Thu 12:30 H6

Potential step experiments on Ag_xPt_{1-x}/Pt(111) surface alloys - the influence of the upper potential limit on surface structure — •Stephan Beckord, Sylvain Brimaud, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm

Ag_xPt_{1-x}/Pt(111) surface alloys exhibit electrochemical and catalytic properties which differ significantly from those of the individual metals. Studies in our institute revealed them as a very promising candidate for the oxygen reduction reaction [1]. To unveil possible restructuring or corrosion processes during the electrocatalytic reaction, which could strongly influence the electrocatalytic characteristics of the surface alloy, we investigated the electrochemical corrosion behavior of structurally well-defined Ag_xPt_{1-x} surface alloys on Pt(111) with different Ag contents. The surface alloys were prepared under ultrahigh vacuum (UHV) conditions and structurally characterized by STM before and after electrochemical investigation. Electrochemical characterization was performed in a flow cell set up, which also allows measuring the dissolution of surface atoms during corrosion by a collector electrode. Additionally the corroded surfaces were electrochemically characterized by basic cyclic voltammetry (BCV) in supporting electrolyte (0.5 M H_2SO_4). We demonstrate that the sensitivity of the surface structure towards corrosion depends sensitively on the surface composition. The role of Pt atoms for stabilizing the Ag surface atoms is discussed.

[1] S. Beckord, S. Brimaud, R.J. Behm, *ORR on Structurally well-defined Ag_xPt_{1-x}/Pt(111) surface alloys* (in preparation)

O 82.10 Thu 12:45 H6

Surface engineering of nanomaterials for electrochemical energy conversion and storage — •Min Zhou and Yong Lei — Institute for Physics and IMN MacroNano*, Ilmenau University of Technology, Ilmenau 98693, Germany

In view of the worldwide energy challenge in the 21st century, the electrochemical technologies have received considerable attention for energy conversion (i.e. photoelectrochemical water splitting) and storage (i.e. secondary ion battery). Nearly all chemical transformations related to energy conversion and storage take place at the surfaces and interfaces between electrode and electrolyte. Hence, surface engineering of nanomaterials offers the possibility to optimize the final electrochemical devices. We employ three-dimensional (3D) ordered porous architectures to illuminate the important role of surface science for energy conversion and storage. For example, a 3D ordered macro-mesoporous architecture of BiVO4 is first fabricated through a modified colloidal crystal template method. Superior photocurrent densities are achieved in return for controllable surface-to-volume ratio. This advantage can be further enhanced within the photoelectrodes of faster charge transport. As for electrochemical storage, 3D ordered porous architecture of amorphous TiO2 is chose as a proof-of-concept prototype to illuminate the importance of surface design for rate capability in sodium ion batteries. The enhancement is primarily attributed to effective surface ion availability by increasing the roughness of the electrode surface. Both the results of energy conversion and storage highlight the great significance of surface engineering for energy-related area.

O 83: Heterostructures and Interfaces

Time: Thursday 9:30–13:15 Location: H17

O 83.1 Thu 9:30 H17

Silicon p-n junctions prepared by group-V in-diffusion in CVD ambient — •Agnieszka Paszuk, Oliver Supplie, Marek Duda, Anja Dobrich, Peter Kleinschmidt, Sebastian Brückner, and Thomas Hannappel — Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau, Germany

Integration of III-V materials with Si substrates is promising for high-efficiency tandem solar cells. Preparation of Si bottom cell in MOCVD environment requires control over the doping. Phosphorus (P) in-diffusion into crystalline Si is a complex process, but has been shown suitable to form a working emitter [1,2]. Arsenic (As) in-diffusion on the other hand is interesting since Si surfaces terminated with As enable the prepareation of B-type GaP/Si(111)[3] and As-based planar graded buffer layers. Here, we focus on As and P in-diffusion and its impact on the Si surface (controlled by in-situ reflection anisotropy spectroscopy). Diffusion of As and P into Si is carried out by annealing the substrates under TBAs or TBP. We investigated the diffusion in dependence on duration and temperature of the annealing step, precursor source, reactor pressure and post diffusion annealing. Annealing the Si surface in presence of the precursors results in surface roughening and a disordered surface. Subsequent annealing without precursor supply leads to a re-ordered dimerized surface. [1] E. García-Tabarés et al., 8th International Conference on Concentrating Photovoltaic Systems (2012). [2] R. Varache et al., Energy Procedia 77, 493 (2015). [3] A. Paszuk et al., Appl. Phys. Lett. 106, 231601 (2015).

O 83.2 Thu 9:45 H17

Interfacial Doping of a MoS2 Monolayer in a 2D Heterostructure — •Mahfujur Rahaman[1], Gerd Plechinger[2], Raul D. Rodriguez[1], Christian Schüller[2], Tobias Korn[2], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Technische Universität Chemnitz,09126 Chemnitz, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany

We report on the interfacial doping of the transition metal dichalcogenide MoS2 monolayer in contact with GaSe and graphite (HOPG). Photoluminescence (PL) results suggest that the PL emission of MoS2 monolayer on top of GaSe is dominated by neutral excitons. This is in contrast to MoS2 in contact with HOPG where trions dominate the PL due to n-type doping. Raman spectroscopy investigations indicate e- doping of the MoS2 monolayer on top of HOPG reflected by the change in A1g out-of-plane mode. Finally, the carrier concentration of MoS2 monolayers for both interfaces is quantitatively determined by Kelvin probe force microscopy (KPFM). Our results pave the way for simple, scalable, and patterned doping in order to modify the electrical and optical properties of MoS2 monolayers and other 2D materials by engineering the graphite substrate.

O 83.3 Thu 10:00 H17

Epitaxial growth and conductivity mechanisms of [LaNiO$_3$/LaAlO$_3$]$_{10}$ superlattices — •Haoming Wei, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Exp. Physik II, Germany

LaNiO$_3$ (LNO) is an interesting material exhibiting Pauli paramagnetic metallic behavior in a wide temperature range. New properties can emerge in the LNO-based superlattices (SLs) by modifying the orbital, electronic, and magnetic structure of bulk LNO [1]. We have grown LNO, LaAlO$_3$ (LAO) films, and [LNO (d nm)/LAO (2 nm)]$_{10}$ SLs by plused laser deposition [2]. Sharp reflection high-energy electron diffraction patterns and atomic force microscopy images confirm an atomically flat surface. Reciprocal space maps reveal the in-plane lattice match of the SLs to the substrates. X-ray reflectivity data with strong Bragg reflections indicate abrupt interfaces of SLs with interfacial roughness in the order of one unit cell. A clear quantum confinement effect on the electronic properties including a metal-insulator transition (MIT) of the LNO/LAO SLs is demonstrated for decreasing LNO thickness. Single LNO films and SLs with LNO thickness of 4 nm show metallic behaviour at all temperatures. The SL with 2 nm thick LNO shows MIT due to the quantum interference of electronic waves. Strong localization appears when the LNO thickness of SLs reduced to 1.2 nm and two-dimensional variable range hopping is the main conduction mechanism.

[1] M. K. Stewart et al. J. Appl. Phys. 110, 033514 (2011).

[2] H. M. Wei et al. Appl. Phys. Lett. 106, 042103 (2015).

O 83.4 Thu 10:15 H17

How can band offsets in III-V nanowires be determined correctly by scanning tunneling spectroscopy? — •Philipp Ebert[1], Pierre Capiod[2], Tau Xu[2], Adrian Díaz Álvarez[2], Xiang-Lei Han[2], David Troadec[2], Jean-Philippe Nys[2], Maxime Berthe[2], Liverios Lymperakis[3], Jörg Neugebauer[3], Isabelle Lefebvre[2], Sébastien Plissard[2,4], Philippe Caroff[2,5], Rafal Dunin-Borkowski[1], and Bruno Grandidier[2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]IEMN, CNRS, UMR 8520, Dept. ISEN, 59046 Lille, France — [3]Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [4]CNRS-LAAS, Univ. de Toulouse, 31400 Toulouse, France — [5]Dept. of Electronic Materials Engineering, Australian National University, Canberra, ACT 0200, Australia

Scanning tunneling spectroscopy (STS) allows the determination of band gaps and band offsets at interfaces between different polytypes or materials of III-V semiconductor nanowires (NWs). However, STS is mostly wrongly interpreted in literature: The commonly high step density at the sidewall surfaces of III-V NWs leads to extrinsic surface states that induce a pinning of the Fermi energy within the fundamental band gap. Since the pinning level is different on every polytype/material, the relative band edge positions between different NW segments are extrinsically determined. Therefore, we developed a new methodology to accurately determine band offsets between different NW segments by using a thin overgrown shell with wider band gap, assuring identical pinning of the overgrown and the pure segment.

O 83.5 Thu 10:30 H17

Atomic-Scale Electronic Structures across BiFeO$_3$/La$_{0.7}$Sr$_{0.3}$MnO$_3$ Heterointerfaces — •Ya-Ping Chiu[1,2], Bo-Chao Huang[3], Pu Yu[4], Chia-Seng Chang[3], and Ying-Hao Chu[3,5] — [1]Dept. of Physics, National Taiwan Normal University, Taipei 116, Taiwan — [2]Dept. of Physics, National Sun Yat-sen University, Kaohsiung 804, Taiwan — [3]Institute of Physics, Academia Sinica, Taipei 115, Taiwan — [4]State Key Laboratory of Low-Dimensional Quantum Physics, Dept. of Physics, Tsinghua University, and Collaborative Innovation Center of Quantum Matter, Beijing 100084, China — [5]Dept. of Materials Science and Engineering, National Chiao Tung University, Hsinchu 300, Taiwan

Atomic-level evolution of electronic structures across BiFeO$_3$/La$_{0.7}$Sr$_{0.3}$MnO$_3$ complex oxide heterointerfaces has been demonstrated by cross-sectional scanning tunneling microscopy and spectroscopy in this work. Analysis of scanning tunneling spectroscopy results exploits how the change in the terminated interface brings the influence to the electrostatic configurations across the BiFeO$_3$/La$_{0.7}$Sr$_{0.3}$MnO$_3$ heterointerfaces. Spatially unit-cell-by-unit-cell resolved electronic states at the atomic level reveal that the control of material interfaces at the atomic level determines the ferroelectric polarization in BiFeO$_3$. The precise electronic information therefore provides a clear realization about the electronic state at these complex-oxide heterointerfaces, which is crucial to understand and design a host of novel functionalities at complex oxide heterointerfaces.

30 min. Coffee Break

O 83.6 Thu 11:15 H17

Ultrafast multi-terahertz nanoscopy of strained vanadium dioxide nanobeams — •Markus A. Huber[1], Markus Plankl[1], Max Eisele[1], Robert E. Marvel[2], Fabian Sandner[1], Tobias Korn[1], Christian Schüller[1], Richard F. Haglund[2], Rupert Huber[1], and Tyler L. Cocker[1] — [1]Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics and Astronomy and Interdisciplinary Materials Science Program, Vanderbilt University, Nashville, Tennessee 37235-1807, USA

Long regarded as a model system for studying insulator-to-metal transitions, vanadium dioxide features a rich phase diagram including at least three insulating states and one metallic state. Recently, the effects of strain on the transition temperature and nanoscale domain structure have been brought into focus. In this regard scattering-type near-field microscopy in the multi-terahertz regime [10-100 THz] has been proven to be a valuable tool for imaging the spatial heterogeneity of the transition. However, so far no time-resolved near-field studies have been undertaken. Here, we show the local pump-probe behavior of a single-crystalline vanadium dioxide nanobeam upon near-infrared photoexcitation. We probe with an ultrafast multi-terahertz pulse and see a modulation of the photoconductivity along the c_R-axis of the wire. This modulation qualitatively matches the different switching susceptibilities inside the wire upon thermal heating. We therefore propose that the switching susceptiblity is built into the wire already at room-temperature, most likely by strain.

O 83.7 Thu 11:30 H17

Structural and optical characterization of hybrid ZnO/polymer nanostructures fabricated by spin coating — •Stephanie Bley[1], Alejandra Castro-Carranza[1], Linus Krieg[2], Tobias Voss[2], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen — [2]Institute of Semiconductor Technology, Braunschweig University of Technology, 38106 Braunschweig

Hybrid core-shell nanowires with inorganic ZnO cores and organic p-conductive polymer shells have shown to possess a huge potential for the realization of efficient light-emitting or photovoltaic devices. A controlled deposition of the polymer shell is required to tailor the electronic and optical properties.

We show that spin-coating of planar ZnO layers and nanowires with poly(3,4-ethylenedioxythiophene) (PEDOT) is suitable to form hybrid heterojunctions. A thin polystyrene passivating interlayer is deposited in the hybrid structure. Its thickness is systematically modified to study its impact on defect state passivation, confirmed by the optical and electrical performance of the heterojunction. SEM and TEM characterization of the hybrid ZnO/polymer nanostructures show that conformal coating is possible. PL measurements confirm that the general optical properties of the ZnO have not been significantly changed after the coating process. A reduction of the defect luminescence of the ZnO is found for the passivated samples.

O 83.8 Thu 11:45 H17

Photoelectrochemical investigation of TiO_2-coated InGaN/GaN nanowires under visible light irradiation — •Paula Neuderth[1], Adina Frank[1], Pascal Hille[1], Christian Reitz[2], Jörg Teubert[1], Jörg Schörmann[1], Roland Marschall[3], and Martin Eickhoff[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Gießen, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany — [3]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Gießen, Germany

Composite structures of InGaN/GaN nanowire heterostructures with a thin anatase titania coverage were prepared by combination of molecular beam epitaxy and atomic layer deposition and investigated with respect to their photoelectrochemical properties. The bandgap of InGaN can be adjusted in the visible regime which makes it suitable for solar-driven photocatalytic reactions such as solar water splitting. In these nanocomposite structures an anodic photocurrent under visible excitation was gained. However, the presence of a thin (2 - 10 nm) anatase titania film increases the photocurrent significantly although direct generation of carriers in the titania is not possible. The influence of the titania coating on charge separation, charge transfer and surface recombination will be discussed by comparison to photoluminescence measurements in electrochemical environment.

O 83.9 Thu 12:00 H17

Disorder and Interface Properties in III-N-V-quantum wells — •Sebastian Gies, Sarah Karrenberg, Tatjana Wegele, Phillip Springer, Christian Fuchs, Andreas Beyer, Martin Zimprich, Wolfgang Stolz, Kerstin Volz, Stephan W. Koch, and Wolfram Heimbrodt — Philipps-University Marburg, 35032 Marburg, Germany

Nitrogen containing quantum well (QW) structures are an interesting material for solar cells and lasers. Because of the band anticrossing between the N-impurity and the GaAs conduction band the band gap is pushed towards 1.55 μm. Otherwise N introduces a huge disorder. The influence of this disorder on QW-interfaces (IF) and optical properties is scarcely studied. However, IFs are an important part of any device and influence strongly the charge carrier confinement and the transport properties. We investigate the quaternary Ga(NAsP) pseudomorphically grown on silicon. This material is a promising light source for optoelectronic integration on silicon. The important disorder parameters are revealed using photoluminescence (PL) spectroscopy, while the material's structure is characterized via transmission electron microscopy and X-ray diffraction. The conjunction of these methods allows us to uncover the complex interplay between N-incorporation and optical and structural properties. Furthermore, type-II excitons in (GaIn)As/Ga(NAs)-heterostructures are studied. The conjunction of experiment and microscopic theory allows us not only to determine the band alignment in the heterostructures, but also to directly analyze the influence of the IF on disorder and optical properties.

O 83.10 Thu 12:15 H17

Hybrid structures of semi-metals, excitonic insulators and superconductors — •Dario Bercioux[1,2] and Sebastian Bergeret[1,3] — [1]Donostia International Physics Center (DIPC), E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain — [3]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastian, Spain

Excitonic insulars are a condensate phase of matter investigated since the sixties [1]. They remain so far an elusive phase in solid state systems. Recent experiments on HgTe quantum wells with a width of circa 20 nm [2] hints at their observation. However, there is no common agreement on this point [3]. Combinations of excitonic insulators with superconductors should show evidence of Andreev processes due to the combination of two different type of condensates [4]. Here, we present results for hybrid structures combining semi-metals, excitonic insulators and superconductors and discuss phenomena related to the interplay between the two distinct condensates.

[1] D. Jérome, T. M. Rice, & W. Kohn, W., Phys. Rev. **158**, 462 (1967).
[2] G. M. Minkov, *et al.*, Phys. Rev. B **88**, 155306 (2013).
[3] M. Knap, J. D. Sau, B. I. Halperin, & E. Demler, Phys. Rev. Lett. **113**, 186801 (2014).
[4] F. Dolcini, *et al.*, Phys. Rev. Lett. **104**, 027004 (2010).

O 83.11 Thu 12:30 H17

A functional renormalization group approach for treating interactions in disordered electron systems — •Christian Seiler and Ferdinand Evers — Institut für Theoretische Physik, Universität Regensburg, Deutschland

We propose an approach to treat the effects of interactions in disordered electron systems on a numerical level. The idea is to solve the non-interacting disorder problem for a given disorder realization exactly. We then use the functional renormalization group method to introduce interactions on a perturbative level. In contrast to usual applications of the fRG, we formulate it in terms of the eigenfunctions of the disordered non-interacting Hamiltonian. The main advantage of our approach is that we are able to treat disorder exactly from a numerical point of view, while the fRG enables us to characterize interaction-induced phase transitions that the system undergoes in an unbiased manner. This allows us to study the phase diagram of a model system without being restricted in the strength of the disorder.

O 83.12 Thu 12:45 H17

***Ab initio* Anderson localisation in Si:P** — •Edoardo G. Carnio[1], Nicholas D. M. Hine[1], David Quigley[1,2], and Rudolf A. Römer[1,2] — [1]Department of Physics, The University of Warwick, Coventry CV4 7AL, UK — [2]Centre for Scientific Computing, The University of Warwick, Coventry CV4 7AL, UK

The Anderson metal-insulator transition (MIT) has long been studied, but there is still no agreement on its critical exponent when comparing experiments and theory. In this work, we employ *ab initio* methods to study the MIT that occurs in phosphorus-doped silicon (Si:P) when the density of the dopants is increased. Our strategy consists in using ONETEP, an implementation of linear scaling DFT, to model an effective potential between the P atoms, which is used in a Monte Carlo simulation to randomly distribute the impurities in the host material. We then combine these spatial configurations with the DFT data into an effective tight-binding Hamiltonian for a system of Si:P close to the critical concentration of the MIT. In this way we characterise the MIT in Si:P including the *ab initio* determined possible spatial correlations in P and the electronic interactions between the donated electrons. The extent of the resulting electronic states is characterised by the participation numbers and their scaling.

O 83.13 Thu 13:00 H17

General DFT+NEGF approach for modeling metal-semiconductor interfaces — •daniele stradi[1], umberto martinez pozzoni[2], anders blom[2], mads brandbyge[1], and kurt stokbro[2] — [1]DTU Nanotech, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark — [2]QuantumWise A/S, Freubjergvej 3, Postbox 4, DK-2100 Copenhagen, Denmark

Metal-semiconductor (M-SC) contacts play a pivotal role in a broad range of technologically relevant devices. Still, their characterization remains a delicate issue, as the present understanding relies either on simplified analytical models [1], or on simulations describing the interface using simple slab models [2]. We model realistic M-SC interfaces by using the DFT+NEGF method as implemented in the Atomistix ToolKit (ATK) simulation software [3]. An accurate description of the interface is achieved by using a meta-GGA functional [4], and an effective scheme to account for the presence of doping in the SC side. The present approach has the advantages of (i) treating the system using the appropriate boundary conditions and (ii) allowing for a direct comparison between theory and experiments by simulating the I-V characteristics of the interface. We apply this methodology to an Ag/Si interface relevant for solar cell applications, and test the reliability of traditional strategies [1,2] to describe its properties [5]. [1] Physics of Semiconductor Devices: 3rd edition (Wiley, 2006); [2] Phys. Rev. B 35, 8154 (1987); [3] Atomistix ToolKit version 2015.0, QuantumWise A/S (www.quantumwise.com); [4] Phys. Rev. Lett. 102, 226401 (2009); [5] D. Stradi et al. In preparation

O 84: Scanning Probe Techniques: Method Developments

Time: Thursday 15:00–18:15 Location: S054

Invited Talk O 84.1 Thu 15:00 S054

Radio frequency STM on molecular resonators — •Stefan Müllegger — Johannes Kepler University Linz, Institute of Semiconductor and Solid State Physics, Linz, Austria.

To benefit from both, the superior spatial resolution of scanning tunneling microscopy (STM) and the exceptional energy resolution of magnetic resonance techniques, we developed a spectroscopic radio frequency (rf) STM system [1,2]. It enables the detection [1] and excitation [2] of mechanical vibrations of a new type of nano-mechanical resonator system based on one-dimensional chains of only 4 to 7 weakly coupled small molecules on a Au(111) surface. Rf-STM reveals concerted mechanical oscillations at 51–127 MHz with a chain-length dependence in reasonable agreement with a coupled-oscillator model. Moreover, I discuss the resonant excitation of single nuclear (I) and electronic (J) spins by rf tunneling in individual molecular quantum dots by a novel technique denoted as rf scanning tunneling spectroscopy (rf-STS) [3], enabling single-spin spectroscopy unbound from electromagnetic dipole selection rules [4]. Our rf-STS experiments on magnetic molecular quantum dots have revealed nuclear and electronic spin transitions of individual quantum spins of up to $\Delta I_z = \pm 3$ and $\Delta J_z = \pm 12$ with sub-nanometer spatial resolution. The molecular quantum dots are formed by molecules of the single-molecule magnet bis-phthalocyanato terbium (III) on Au(111) at 5 K.

[1] Phys. Rev. Lett. 112, 117201 (2014). [2] Nanotechn. 25, 135705 (2014). [3] Phys. Rev. Lett. 113, 133001 (2014). [4] arXiv:1510.04804.

O 84.2 Thu 15:30 S054

Co-resonant scanning force microscopy sensors — •Christopher F. Reiche[1], Julia Körner[1], Bernd Büchner[1,2], and Thomas Mühl[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung IFW Dresden — [2]Institut für Festkörperphysik, Technische Universität Dresden

A possible route to enable the detection of very small interaction forces in dynamic mode scanning force microscopy (SFM) is to decrease the spatial dimensions of the cantilever force sensor to reduce its effective spring constant and increase its resonance frequency. However, this approach is limited by the required operational stability of the sensor to avoid snap-ins and the capability of the equipment to still reliably detect the sensor's oscillatory state. By applying a recently developed co-resonant sensor concept [1] to bidirectional scanning force microscopy sensors [2], it is possible to combine the stability and ease-of-detection of a standard SFM cantilever with the high sensitivity of a nanocantilever. Since the measurement signal is still generated by observing changes in the oscillatory state of the standard cantilever, these novel sensors for dynamic mode SFM are still compatible with common SFM equipment. To demonstrate the performance of these sensors, we employed iron filled carbon nanotubes as nanocantilevers to achieve sensitivity to magnetic stray fields. A comparison of experimental results to calculated data reveal a signal increase by three orders of magnitude compared to standard force sensors.
[1] C.F. Reiche, J. Körner et al., Nanotechnology 26 (2015) 335501
[2] C.F. Reiche et al., New J. Phys. 17 (2015) 13014

O 84.3 Thu 15:45 S054

Effect of amplitude on bimodal frequency modulation atomic force microscopy with small amplitudes in ambient conditions — •Dominik Kirpal[1], Hiroaki Ooe[2], Daniel Wastl[1], Alfred J. Weymouth[1], Toyoko Arai[2], and Franz J. Giessibl[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Natural Science and Technology, Kanazawa University, Kanazawa, Japan

Bimodal atomic force microscopy (AFM) is usually performed with the first flexural mode excited at a large amplitude to maintain a stable oscillation, and the second mode excited at a small amplitude to be sensitive to short-range interactions. A stiff cantilever, such as the one provided by a qPlus sensor, can be used to perform bimodal AFM with small amplitudes in both flexural modes. We calculated the piezoelectric sensitivity of the qPlus sensor in the second flexural mode and imaged KBr(100) in ambient conditions to determine the ideal amplitudes for atomic resolution with bimodal AFM. The highest signal-to-noise ratio is achieved if the total vertical displacement of the tip in each cycle is less than the thickness of a single hydration layer.

O 84.4 Thu 16:00 S054

Force reconstruction with multifrequency kernel spectroscopy — •Daniel Platz[1,2], Daniel Forchheimer[2,3], Erik A. Tholen[3], John E. Sader[4], and David B. Haviland[2] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, D-01187 Dresden, Germany — [2]KTH Royal Institute of Technology, Albanova University Center, SE-114 19 Stockholm, Sweden — [3]Intermodulation Products AB, Landa Landavägen 4193, SE-823 93 Segersta, Sweden — [4]The University of Melbourne, Victoria 3010, Australia

The object of interest in dynamic atomic force microscopy (AFM) is the interaction force between a sample surface and the tip of an oscillating cantilever. However, the measured data in AFM do not describe this interaction force directly but rather describe properties of the cantilever motion like amplitudes, phase or frequency shifts. Each AFM mode requires extensive modeling to link the measured data and physical properties of the interaction force. Here, we present a general method, called multifrequency kernel spectroscopy (MKS), for interpreting measured AFM data. The method allows for a clear measurement of the "amount of information" in AFM data and a quantitative reconstruction of the interaction force for any AFM mode. To demonstrate the capabilities of MKS we use it to unambiguously separate long and short range forces in multifrequency magnetic force microscopy and reconstruct the tip-sample interaction force from amplitude-modulated AFM measurements.

O 84.5 Thu 16:15 S054

The effect of non-ideal tunneling current amplifiers on force measurements — •Nirmalesh Kumar Sampath Kumar, A. J. Weymouth, V. Junk, F. Huber, and F. J. Giessibl — University of Regensburg, Regensburg, 93053, Germany

Measurements of the tunneling current are performed with a current-to-voltage converter typically implemented by returning the output of an operational amplifier with a resistor in the Mega- to Giga-Ohm range to the inverting input. With the sample is attached to inverting input, and the non inverting input at ground, an ideal operational amplifier would maintain the sample at ground. A real operational amplifier, however, has finite internal impedance and finite gain. This has been shown to affect STM measurements when the internal resistance of the operational amplifier starts to be on the same order of magnitude as the resistance of the tunneling junction. [1]

We have observed that the presence of the current-to-voltage converter can have a profound effect upon the excitation required to oscillate the cantilever. A phase shift between the non-ideal virtual ground and the cantilever oscillation can account for energy either being pumped into or drained from the cantilever as it oscillates. In this contribution, we discuss our observations and this effect in more detail.

References [1] L. Olesen et al. Phys. Rev. Lett. 76, 1485 (1996)

O 84.6 Thu 16:30 S054

high frequency transmission to a junction of a scanning tunneling microscope — •marie hervé, moritz peter, and wulf wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

We report on an easy method to calibrate the transmission of radio-frequency (rf) voltages to the tunneling junction of a scanning tunneling microscope. The transmission strongly depends on frequency, as the cabling shows frequency dependent damping and the impedance mismatch between the cable and the tunneling junction induces reflections. To first order, the current-voltage characteristic of the junction induces a rf tunneling current of the same frequency as the rf voltage. Omnipresent non-linearities of the current-voltage characteristic of the junction to second order, however, generates an additional rectified DC current. A direct comparison between this current and the second derivative of the current-voltage curve allows to determine the rf transmission to the tunneling junction. The transmission data up to 2 GHz were used to compensate the rf damping such that at every frequency a constant amplitude at the tunneling junction could be realized expanding the bandwidth of the experiment from less than 100

MHz to 2 GHz [1].

[1] M. Hervé, M. Peter, and W. Wulfhekel, Appl. Phys. Lett. 107, 093101 (2015)

O 84.7 Thu 16:45 S054

Imaging of 2D electronic structures with Intermodulation — •Riccardo Borgani[1], Erik A. Tholén[2], and David B. Haviland[1] — [1]Nanostructure Physics, KTH Royal Institute of Technology, Stockholm, Sweden — [2]Intermodulation Products AB, Segersta, Sweden

We present a Scanning Probe Microscopy (SPM) technique to image the contact potential difference (CPD) between the tip of a conducting cantilever and the sample surface. A multifrequency drive is used to probe the nonlinear electrostatic force and extract the CPD from the intermodulation signals close to the cantilever resonance. This measurement scheme allows for a very high signal to noise ratio and excellent lateral resolution, and it eliminates the DC feedback to null CPD, used on all other types of Kelvin Probe Force Microscopy. The absence of a DC bias is of particular importance with those samples where electrical doping could alter the properties under investigation. We present a theoretical derivation of the technique, as well as it's application for high-resolution imaging of mono- and multi- layer graphene and graphene nano-ribbons, and patterned two-dimensional electron gas devices.

Reference

R. Borgani, D. Forchheimer, J. Bergqvist, P.-A. Thorén, O. Inganäs, and D. B. Haviland, Appl. Phys. Lett. 105, 143113 (2014).

O 84.8 Thu 17:00 S054

A quantitative tool to measure nanoscale electrostatic potentials — •Matthew F. B. Green[1,2], Christian Wagner[1,2], Philipp Leinen[1,2], Thorsten Deilmann[3], Peter Krüger[3], Michael Rohlfing[3], Ruslan Temirov[1,2], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology — [3]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster

Interactions between nanoscale objects on surfaces are dominated by the van der Waals and electrostatic contributions. The ability to characterize the electrostatic field on a surface would therefore be a valuable tool for many areas of nanoscience research. Recently we presented a technique called scanning quantum dot microscopy (SQDM), whereby local electrostatic potentials on surfaces can be measured quantitatively and in three dimensions. By registering the charging events of a single molecule weakly hybridized to an nc-AFM tip, acting as a QD, the quadrupole potential of a single molecule and the dipole potential of a single ad-atom were investigated. In addition we demonstrated the remarkable sensitivity of SQDM by probing an ad-atom from 6 nm away [1]. We now present a quantitative model of the charging dynamics based on single electron box theory [2], taking the orbital hybridization and junction geometry into account. By fitting the model to experimental data, we show how the system parameters affect the way that the charging manifests itself in the frequency shift signal.

O 84.9 Thu 17:15 S054

Quantitative mapping of magnetic stray fields by dynamic mode magnetic force microscopy — Christopher F. Reiche[1], •Clemens Gütter[1], Silvia Vock[1], Volker Neu[1], Bernd Büchner[1,2], and Thomas Mühl[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung IFW Dresden — [2]Institut für Festkörperphysik, Technische Universität Dresden

Dynamic mode magnetic force microscopy (MFM) is a successful method to study magnetic stray fields of samples with high spatial resolution. Quantitative approaches based on frequency modulation measurements and a point probe approximation for the magnetic tip can supply information about the first or the second order spatial derivative of the magnetic stray field of a sample. However, often it would be favorable to know the more fundamental stray field itself. Here, we demonstrate a technique that enables the measurement of one component of the magnetic stray field of a sample in real space. This technique is based on the integration of frequency shift signal maps gathered at different measurement heights. It employs calibrated iron filled carbon nanotube magnetic tips with monopole-like characteristic [1]. While this technique has some requirements on the sample it does not need any special kind of MFM equipment. The viability of this approach was validated by measurements on a well-characterized Pt/Co magnetic multilayer sample. For such a sample it is possible to calculate its magnetic stray field based on an effective magnetic surface charge pattern approach and compare it to the measured results.

[1] F. Wolny et al., Nanotechnology 21 (2010) 435501

O 84.10 Thu 17:30 S054

Tip-enhanced Raman spectroscopy: comparison between AFM and STM feedback mechanism performance — •Jana Kalbacova, Raul D. Rodriguez, Axel Fechner, and Dietrich R.T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Tip-enhanced Raman spectroscopy (TERS) is a relatively young technique, with the first experimental reports around the year 2000. This technique combines features of two distinct methods - Raman spectroscopy that can e.g. provide details on the chemical composition of a sample, while the metallic tip acts as a nano-antenna enhancing the sample signal only beneath the tip apex. In this way, the chemical information can be resolved at the nanoscale. The way to control the position of the tip apex is the feedback mechanism of the scanning probe microscope. In this contribution, we first review the pros and cons of the atomic force microscopy (AFM) and scanning tunnelling microscopy (STM) feedback loop in TERS. For experimental part of this comparative study, we prepared a sample comprised of single-walled carbon nanotubes and graphene oxide deposited on a gold substrate. An etched gold tip was employed for TERS imaging in both modes. We demonstrate TERS in ambient conditions with sub-10 nm spatial resolution for both approaches (AFM and STM) showing the availability of various working conditions that can be chosen to accommodate different samples with STM, as a feedback loop, displaying better spatial resolution.

O 84.11 Thu 17:45 S054

Quantitative description of light-excited scanning tunneling spectroscopy — •Michael Schnedler, Verena Portz, Phillip Weidlich, Rafal Dunin-Borkowski, and Philipp Ebert — Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The efficiency of solar cell and optoelectronic devices is closely connected to the nanoscale distribution of charge carriers. In order to understand the physical processes involved at the atomic scale, the materials need to be investigated simultaneously under illumination and with atomic resolution. Photo-excited scanning tunneling spectroscopy (STS) is ideally suited to probe the illumination-induced local surface photo-voltage, band bending, carrier concentration, and the electrostatic potential distribution with atomic resolution. For a quantitative analysis, particularly of the local charge carrier concentration, a fundamental physical understanding of the photo-excited tunneling spectra is needed. We will present a new theoretical model of photo-excited STS that incorporates a fully three dimensional solver for both, the electric field and the (intrinsic and photo-excited) carrier concentrations near the semiconductor's surface. In order to take into account both, the tip induced band-bending and the photo-excited carrier concentration, we present a modification of the tunnel current model of Feenstra and Stroscio by introducing Quasi-Fermi levels.

O 84.12 Thu 18:00 S054

Application of Photothermal Expansion for Optical Absorption Mapping at the Nanoscale — •Teresa Isabel Madeira[1], Raul David Rodriguez[2,3], Yuvaprasad Ravikumar[2], Harsha Shah[2], Eugene Bortchagovsky[4], and Dietrich RT Zahn[2,3] — [1]BioISI-Department of Physics-Faculdade de Ciencias-Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal — [2]Semiconductor Physics-Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [3]cfaed-TU Dresden — [4]V. Lashkarev Institute of Semiconductor Physics of NASU, pr.Nauki 41, Kiev 03028, Ukraine

We demonstrate photothermal expansion can be used to obtain images of nanostructured semiconductor materials such as GaSe flakes on graphite and carbon nanotubes on SiO_2 in ambient conditions with high sensitivity and spatial resolution. The principle behind is the detection of the mechanical force exerted on an atomic force microscopy (AFM) tip by the thermal expansion of the materials excited with pulses of optical radiation, taking advantage of the different absorption properties between substrate and sample. Characterization of semiconductor nanostructures, with a bandgap in the optical range enables the use of cw lasers chopped and synchronized with the resonance frequency of custom-made fully metallic cantilever AFM Au tips. The spatial resolution achieved by the synchronization procedure described is indeed in the nanometer range below 60 nm, and by taking advantage of the difference between optical absorption and thermal coefficients material contrast can be achieved. The optimal conditions to make the most of this technique are also discussed.

O 85: Organic-Inorganic Systems IV: Electronic Structure

Time: Thursday 15:00–18:00 Location: S051

Invited Talk O 85.1 Thu 15:00 S051

Electrostatic Design of Organic Materials and Hybrid Interfaces — •Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010-Graz, Austria

In hybrid organic/inorganic interfaces collective electrostatic effects often determine electronic properties like the relative alignment of electronic states, adsorption-induced changes in the work-function, XPS shifts and ballistic transport properties. Here, we suggest ways of intentionally employing these effects for realizing new types of electrostatically designed nanoscopic materials. This includes the development of a modular and versatile toolbox for realizing complex interfacial structures like monolayer quantum-cascades or quantum-well structures. It also comprises the use of polar adsorbates on layered van-der Waals bonded materials like graphene or layered semiconductor structures with the aim of locally concentrating charge carriers for an adsorbate-driven patterning of conductive channels. Finally, I will address possibilities for electrostatically designing the energy landscape of self-assembled three-dimensional organic networks with possible applications in charge carrier separation or carrier injection.

O 85.2 Thu 15:30 S051

Electronic structure of charge transfer salts: application of self-interaction corrected density functional theory — •Torsten Hahn[1], Torsten Hahn[2], and Torsten Hahn[2] — [1]Institute for Theoretical Physics, TU Freiberg, 09599 Freiberg, Germany — [2]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

We present our experimental and theoretical results on novel Picene/F4TCNQ and Manganese-Phthalocyanine/F4TCNQ donor / acceptor systems. We apply the recently developed Fermi-orbital based approach for self-interaction corrected density functional theory (FO-SIC DFT) to these materials and compare the results to standard DFT calculations [1,2,3]. Further we compare the theoretical results with experimental data obtained by photoemission spectroscopy. We focus our analysis on the comparison of orbital eigenvalues, ionization potentials and the magnitude of the ground state charge transfer. We show that for weakly bound donor / acceptor systems the FO-SIC approach delivers results closer to experiment compared to standard DFT calculations.

[1] T. Hahn et al., J. Chem. Phys. (accepted: AIPID 029546JCP).

[2] M. R. Pederson, A. Ruzsinszky, and J. P. Perdew, J. Chem. Phys. 140, 121103 (2014).

[3] M. R. Pederson, J. Chem. Phys. 142, 064112 (2015).

O 85.3 Thu 15:45 S051

Structural and electronic properties of organic charge-transfer complexes on Ag(111) — •Kathrin Müller[1,2], Nico Schmidt[1], Michael Grunst[3], Rene Riedel[3], Milan Kivala[3], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Department of Chemistry and Pharmacy, University Erlangen-Nürnberg, Germany

The use of organic molecules in electronic devices is gaining increasing interest due to their low cost, flexibility and easy processability. However, organic molecules often show weak intermolecular interactions limiting the electron mobility of organic films. One way to overcome these problems is the use of complementary molecules, which exhibit a strong intermolecular interaction. We employ molecules with complementary functional groups as well as complementary building blocks, e.g. by using electron rich and electron poor building blocks. In this work, we studied the self-assembly and the electronic properties of two molecules containing cyano- and methoxy-groups, respectively, on a Ag(111) surface. The cyano-functionalized molecule exhibits a high electron affinity, while the other one shows a low ionization potential. The investigations of the structural and electronic properties of the individual species as well as the mixed layer were carried out by scanning tunneling microscopy and spectroscopy, X-ray and ultraviolet photoelectron spectroscopy and low-energy electron diffraction. We found that the electronic properties of the mixed layer are changed with respect to the assemblies containing one molecular species.

O 85.4 Thu 16:00 S051

Electronic Structure of TIPS-Pentacene on Au(111) — •Arnulf Stein and Petra Tegeder — Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Germany

Functionalized Oligoacenes have moved into the field of view for applications in organic electronic devices during the last years. One representative of this group of organic semiconductors is the triisopropylsilylethynyl-pentacene (TIPS-Pc) which stands out because it combines solubility, self-assembly into π-stacked arrays to enhance intermolecular orbital overlap [1] and vacuum processability [2]. Furthermore it can undergo a singlet fission process [3], which is one possibility to overcome the theoretical Shockley Queisser - Limit. We investigated the TIPS-Pc/Au(111) interface by means of two-photon-photoemission (2PPE) which is one of the most powerful tools to elucidate electronic structures and dynamics of optically excited states at interfaces and within thin films.

[1] J.E. Anthony *et al.*, JACS, 123, 9482 (2001).

[2] A. Gnoli *et al.* J. Phys. Chem. C, 118, 22522 (2014).

[3] A. J. Musser *et al.* Nat. Phys. 11, 352 (2015).

O 85.5 Thu 16:15 S051

Charge transport across interfaces between metals and disordered-semiconductors — Philipp Breitegger[1], Markus Krammer[1], Chris Groves[2], and •Karin Zojer[1] — [1]Institute of Solid State Physics and NAWI Graz, Graz University of Technology, Graz, Austria — [2]School of Engineering and Computing Sciences, Durham University, United Kingdom

Injection of charges from the metal contacts into organic semiconductors, i.e., de facto insulators, is crucially determining the performance of organic devices. Reaching an in-depth understanding of fundamental processes occurring when a steady-state electric current passes the interface, is an indispensable step towards truly active control of charge transport, e.g., by manipulating both interface and semiconductor via intentional doping. To conceive a model being strictly based on the injection barrier, the shape of the density of states, and the external bias, we utilize Kinetic Monte Carlo simulations to identify conditions leading to ohmic or space charge limited currents, i.e., currents being exclusively determined by the semiconductor. A fraction of charges entering the semiconductor is immobilized at the interface such that the Fermi level becomes aligned with the semiconductors transport energy at the interface. Owing to this alignment, further carriers are injected resonantly and contribute to the current. On the basis of these findings, we formulate a necessary condition to obtain bulk-limited current irrespective of the injection barrier.

O 85.6 Thu 16:30 S051

Characterizing Charge-Transfer Effects at Metal/Organic Interfaces by means of Two-Photon Photoemission — •David Gerbert and Petra Tegeder — Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Deutschland,

Further progress in the field of organic electronic devices requires a fundamental understanding of metal/molecule interactions at the interface between organic semiconducting materials and metal electrodes. These metal/molecule interactions lead to an energetic realignment, including the formation of new states and even bands, which may act as a basis for a improved device performance [1].Two-photon photoemission (2PPE) is a powerful tool which enables the observation of occupied and unoccupied electronic states directly at the interface. Additionally 2PPE experiments can be performed in a time-resolved or angle-resolved manner to gain insights into dynamics of optically excited electronic states and possible delocalized charge-carriers.

In this talk I will show recent results of different adsorbate/metal interfaces indicating adsorption-induced energetic realignment and band formation.

[1] M. Wießner et al., Nat- Commun. 2013, 4, 1514.

O 85.7 Thu 16:45 S051

Excitation dynamics at the PTCDA/TiOPc heterointerface on Ag(111) — •Alexander Lerch[1], Frederik Schiller[1,2], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — [2]Centro de Física de Materiales, San Sebastian, Spain

The charge carrier transport across metal/organic and organic heterointerfaces was investigated by means of time-resolved two-photon photoemission (2PPE). We deposited well defined layers of perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) on top of titanylphthalocyanine (TiOPc) on an Ag(111) substrate as model system. An optical parametric oscillator (OPO) provided tuneable pump pulses with photon energies ranging from 1.6 to 2.5 eV. Excitons in PTCDA and TiOPc were excited selectively and the subsequent charge transfer to the metal was monitored by photoemission with 4.3 eV probe pulses. An unoccupied interface state lying 0.3 eV above the Fermi energy arises at the TiOPc/Ag(111) interface. Although a second TiOPc layer is used to form the organic heterostructure and separate the PTCDA from the silver, we observe a resonant enhancement of the interface state for 2.3 eV pump photons, which corresponds to the excitonic HOMO-LUMO transition in PTCDA. We find a time delayed transfer of electrons from PTCDA across the TiOPc layers into the interface state on the time scale of approximately 200 fs. Our results indicate the importance of the interface state for charge carrier dynamics at heterostructures close to the Ag(111) surface.

O 85.8 Thu 17:00 S051

Nanoscale Imaging of Charge Carrier and Exciton Trapping at Structural Defects in C_{60} Films — •Christoph Grosse[1], Olle Gunnarsson[1], Pablo Merino[1], Klaus Kuhnke[1], and Klaus Kern[1,2] — [1]Max-Planck-Institut fürr Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]École Polytechnique Fèdérale de Lausanne, 1015 Lausanne, Switzerland

Charge carrier and exciton trapping in organic semiconductors crucially determine the performance of organic (opto-) electronic devices, such as organic field-effect transistors, light-emitting diodes, or solar cells. However, the microscopic origin of the relevant traps generally remains unclear, as most spectroscopic techniques are unable to probe the electronic structure of individual traps and the morphological structure causing them. Here, we employ low-temperature scanning tunneling microscopy (STM) and tunneling spectroscopy as well as tight-binding calculations derived from ab initio calculations to image the localized electronic states arising at structural defects in thin C_{60} films (<10 ML). The spatially and spectrally resolved STM-induced luminescence at these states reveals an enhanced radiative decay of excitons, which is interpreted in terms of the local symmetry lowering and the trapping of excitons by an X-traps. The combined mapping of the STM-induced luminescence, electronic structure, and morphology thus provides new insights into the origin and characteristics of individual exciton traps in organic semiconductors and opens new avenues to study charge carrier and exciton dynamics at molecular scales.

O 85.9 Thu 17:15 S051

Theory of excitation transfer in hybrid inorganic/organic systems: Coulomb transfer between semiconductor and molecular layers — •Judith Specht[1], Eike Verdenhalven[1], Sverre Theuerholz[1], Andreas Knorr[1], Marten Richter[1], Bjoern Bieniek[2], and Patrick Rinke[2,3] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Aalto University, Aalto, Finland

Hybrid inorganic/organic systems form a novel class of composite materials with interesting optoelectronic properties. Due to the Coulomb interaction, Wannier-exciton like states in an inorganic semiconductor nanostructure are coupled to Frenkel excitons occurring in organic materials. The considered structure consists of a thin, highly ordered molecular film adsorbed on a semiconductor quantum well. Based on a density matrix theory, we study the Förster-type non-radiative excitation transfer across the hybrid interface. The microscopic input parameters are taken from ab initio caculations for ladder-type quarterphenyl (L4P) molecules on the ZnO(10$\bar{1}$0) surface [1]. As a consequence of microscopic momentum selection rules, the coupling strength between the two constituents varies for different coverage densities of the semiconductor surface with molecules.Our findings can be used for optimizing the energy transfer efficiency by modifying the geometry of the hybrid structure.
[1] Verdenhalven et al., Phys. Rev. B **89**, 235314 (2014).

O 85.10 Thu 17:30 S051

Photo Switching the Optical Nonlinear Response of a Fulgimide Functionalized Silicon Surface — •Marc Hänsel[1], Christoph Barta[2], Karola Rück-Braun[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — [2]Institut für Chemie, Technische Universität Berlin, Germany

Fulgimides are a group of molecules which undergo a ring closing and opening reaction under illumination with UV and visible light. They can retain their photochromic properties after binding to a silicon surface by a well-chosen linker molecule. Due to the large hyperpolarizability of the molecules the nonlinear optical (NLO) properties of the surface can be controlled by illumination with light. The samples were investigated with second harmonic generation (SHG), taking advantage of the symmetry of the substrate, which generates no SHG signal. We will show that a controlled photoinduced reversible change of the NLO properties of an indolylfulgimide functionalized silicon surface is possible.

O 85.11 Thu 17:45 S051

Reversible photo-switching of spiropyran molecules in direct contact with a single crystal — •Fabian Nickel, Matthias Bernien, Kai Kraffert, Dennis Krüger, Lucas M. Arruda, Lalminthang Kipgen, and Wolfgang Kuch — Institut für Experimentalphysik, Freie Universität Berlin, 14195 Berlin, Germany

The photochromic isomerization of molecules in direct contact with solid surfaces plays an important role for the further miniaturization of electronic devices. A good candidate for this purpose is spiropyran (SP). SP can be switched from a closed form to an open form (merocyanine, MC) by UV light and reversibly back by visible light. In nitro-spiropyran, however, the backreaction was found to be quenched on surfaces [1]. The modification of the end group from nitro- to naphtho-spiropyran leads to a lower electric dipole moment in the open form, which might favor switching back to the open form on a surface. In-situ x-ray absorption fine structure (NEXAFS) measurements at the nitrogen and oxygen edges prove and quantify the photoisomerization of these molecules on a Bi(111) surface. Illumination by UV light leads to an efficient switching to the open MC form of the molecule and, furthermore, a determination of the energy barriers of the photo-excited and metastable states becomes possible by temperature-dependent measurements. Visible light triggers the relaxation back to the closed SP form, thus offering full reversible control of the isomerization in direct contact with a single crystal surface.

This work is supported by the DFG through Sfb 658.

[1] Piantek et al. J. Am. Chem. Soc. 131, 12729 (2009).

O 86: Ultrafast Surface Dynamics I

Time: Thursday 15:00–18:00 Location: S052

O 86.1 Thu 15:00 S052

Imaging ultrafast photo-induced dynamics in semiconducting polymer films with time-resolved photoemission electron microscopy — •Andreas Neff and Katrin Siefermann — Leibniz-Institute of Surface Modification, Leipzig, Germany

Organic semiconductors have great potential for applications in optoelectronic devices. By now, it is well established that the performance of devices critically depends on the detailed morphology of the organic semiconducting films [1]. However, a profound understanding of the correlation between morphology and (photo)physical properties is still missing, and this remains a key challenge to overcome technological hurdles in the field.

We address this challenge with a combination of a photoemission electron microscope (PEEM) and a femtosecond laser system. With this setup, we image the morphology of films of organic semiconductors, in particular the size and orientation of crystallites, with a lateral resolution of ∼100 nm. Ultrafast pump-probe experiments allow us to image photo-induced dynamics with a temporal resolution of 150 fs and a lateral resolution of ∼100 nm. Here, we present results from the ultrafast exciton decay dynamics in P3HT (Poly(3-hexylthiophen-2,5-diyl)) films. We find that these decay dynamics are - as expected but not previously detectable - not the same for all locations on the sample. These results demonstrate the potential of time-resolved PEEM to address key questions with regard to the relationship between nanoscale morphology of organic semiconductors and photo-physical properties.

[1] Y. Diao et al., Nat. Commun. 6, 7955 (2015).

O 86.2 Thu 15:15 S052

Electron-lattice interactions in gold clusters and islands studied with ultrafast electron diffraction — •Thomas Vasileiadis[1], Dawn Wells[2], Lutz Waldecker[1], Roman Bertoni[1], Richard Palmer[2], and Ralph Ernstorfer[1] — [1]Department of Physical Chemistry, Fritz-Haber-Institut, Fardayweg 4-6 14195 Berlin Germany — [2]Nanoscale Physics Research Laboratory, School of Physics and Astronomy, University of Birmingham, Edgbaston Birmingham B15 2TT

Metallic nanoclusters possess a number of functionalities including catalytic activity and fluorescent emission that are absent from their bulk counterparts. In order to shed light into these confinement-induced properties, an in-depth understanding of the interactions between the subsystems of charge carriers and the lattice is essential. For this purpose we employ ultrafast electron diffraction to study size-selected gold nanoclusters and nanoislands supported by two-dimensional substrates. After laser excitation of the electronic subsystem, the evolution of lattice temperature and expansion can be probed from the intensity and position of diffraction peaks respectively. The so-called two-temperature-model allows for a quantification of how strongly the lattice couples to electronic excitations. The results are compared with thin films of gold that approach the bulk limit. We also discuss the effects that possibly rise due to electronic and vibrational coupling with the substrate.

O 86.3 Thu 15:30 S052

Non-thermal phonon distribution in out-of-equilibrium aluminium — •Lutz Waldecker[1], Roman Bertoni[1], Jan Vorberger[2], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft — [2]Max-Planck-Institut für Physik komplexer Systeme

The interaction between electrons and lattice vibrations is central to both ground state as well as out-of-equilibrium properties of solids. We apply an approach based on femtosecond electron diffraction to retrieve these interactions in laser-excited aluminium at various excitation conditions by measuring the temporal evolution of the atomic mean squared displacement. The data is described with a refined version of the two-temperature model, which is inspired by ab initio theory calculations and allows for transient non-thermal phonon distributions. Our work suggests that assuming thermal phonon distributions, i.e. employing a two-temperature model, can lead to systematic errors in the interpretation of time-resolved experiments.

O 86.4 Thu 15:45 S052

Nonequilibrium electron dynamics in laser excited copper, silver and gold — •Sebastian Weber and Baerbel Rethfeld — Fachbereich Physik und Forschungszentrum OPTIMAS, TU Kaiserslautern, Germany

After excitation with an ultrashort laser pulse, the electrons in a metal are in a strong nonequilibrium state. During thermalization, they interact also with the lattice, transferring energy to the phonons. On the basis of complete Boltzmann-type collision integrals, a method allowing to treat materials with an arbitrary density of states has been developed [Phys. Rev. B 87, 035139 (2013)]. This method provides insights into the response of different material classes to ultrafast laser excitation. Here we focus on the study of noble metals which possess characteristic densities of states with an elevated area at a certain distance below the Fermi edge. The results show the thermalization of the electrons within a few femtoseconds. However, electron-phonon coupling hinders the electrons' complete thermalization as long as the temperature of both subsystems differ from each other.

O 86.5 Thu 16:00 S052

Ultrafast Optical Control of the Electronic Properties of ZrTe5 — •Alberto Crepaldi[1], Giulia Manzoni[2], Andrea Sterzi[2], Timo Kuhn[3], Luca Gragnaniello[3], Gabriel Autès[4], Michele Diego[2], Federico Cilento[1], Michele Zacchigna[5], Philippe Bugnon[4], Arnaud Magrez[4], Helmuth Berger[4], Mikhail Fonin[3], Oleg Yazyev[4], Marco Grioni[4], and Fulvio Parmigiani[1,2] — [1]Elettra-Sincrotrone Trieste, Italy — [2]Universitá degli Studi di Trieste, Italy — [3]University of Konstanz, Germany — [4]EPFL, Switzerland — [5]C.N.R.-I.O.M., Italy

ZrTe5 has recently attracted considerable interest owing to some unique, albeit only partially understood, properties. The electrical resistivity exhibits a peak at a temperature where the nature of the charge carriers changes from holes to electrons. The observed negative magneto-resistance has been attributed to the presence of Dirac particles, either three-dimensional or two-dimensional and spin-polarized. Our time and angle-resolved photoelectron spectroscopy (tr-ARPES) study has addressed the origin of the anomalous transport behavior of ZrTe5, while showing the possibility to control the electronic properties of this material via sub-ps IR laser pulses. These observations open the way to the exploitation of ZrTe5 as a platform for magnetoelectric optical and thermoelectric transport applications. Finally, by combining ab initio calculations, ARPES and scanning tunneling microscopy (STM) we are contributing to shed light on the topological nature of ZrTe5, which is shown to be close to transition between strong and weak topological insulator phases.

O 86.6 Thu 16:15 S052

Two-Photon Photoemission on ultrathin CoO films — •Mathias Albrecht[1], Konrad Gillmeister[1], Cheng-Tien Chiang[2,1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Max-Planck-Institute für Mikrostrukturphysik, Halle (Saale), Germany

Unoccupied electronic states of ultrathin cobalt oxide films grown on Ag(001) are studied by time- and angle-resolved two-photon photoemission (2PPE) spectroscopy. With pump/probe photon energies of 4.2 and 1.8 eV, a series of states at 3.55, 3.87 and 4.00 eV above E_F could be identified. The strongest feature at 3.55 eV is assigned as $n = 1$ image potential (IP) state of ultrathin CoO films due to its characteristic parabolic dispersion. At the $\overline{\Gamma}$ point, the IP state has a lifetime of approximately 35 fs. Additionally to the IP states near the vacuum level, an unoccupied CoO conductive band state has been found at 2.3 eV above E_F with a lifetime below 30 fs. Our results are discussed with the theoretical electronic structure of CoO and compared with results for NiO films.

O 86.7 Thu 16:30 S052

Hot electron-spin gas drives ultrafast spin density wave transition in Cr — •Chris Nicholson[1], Claude Monney[2], Robert Carley[3], John Bowlan[4], Björn Frietsch[5], Martin Weinelt[5], and Martin Wolf[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]University of Zurich, Switzerland — [3]European XFEL GmbH, Germany — [4]Los Alamos National Laboratory, USA — [5]Freie Universitaet Berlin, Berlin, Germany

Transitions to magnetically ordered states are characterised by an order parameter, defined in the (equilibrium) adiabatic limit. However, it is an open question how the order parameter develops on ultrafast timescales following abrupt excitation by an ultrashort laser pulse and if a general description of such ultrafast phase transitions in terms of a theoretically determined order parameter is still possible [1].

We exploit the energy and momentum selectivity of time- and angle-resolved photoemission spectroscopy to address the ultrafast dynamics of the antiferromagnetic SDW photoexcited in epitaxial thin films of chromium. We reveal we are able to quantitatively extract the evolution of the SDW order parameter through the phase transition, which follows the electronic temperature. We observe the complete destruction of antiferromagnetic order on a sub-100fs time scale, which implies that a quasi-equilibrium between electron and spin systems develops on an ultrashort time scale and drives the spin density wave transition in chromium.

[1] P. Beaud et al. Nat. Mater. 13, 1 (2014)

O 86.8 Thu 16:45 S052

Dynamics of photoexcited quasiparticles across the full Brillouin zone of optimally doped $Bi_2Sr_2Cu_2O_{8+\delta}$ probed by time- and angle-resolved XUV photoemission spectroscopy — •Kerstin Hanff[1], Lexian Yang[2], Lars-Philip Oloff[1], Florian Diekmann[1], Gerald Rohde[1], Ankatrin Stange[1], Michael Bauer[1], and Kai Rossnagel[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel Germany — [2]Physics Department, Tsinghua University, Beijing 100089, People's Repuplic of China

Conventional angle-resolved photoemission spectroscopy (ARPES) has added tremendously to our understanding of the electronic and superconducting properties of the cuprates, through direct measurement of the momentum-dependent electronic structure, spectral function, and order parameter. Femtosecond time-resolved ARPES has recently provided a complementary direct view on the momentum-dependent dynamics of quasiparticles (QPs) and Cooper pairs. Here, we present the results of time-resolved ARPES on optimally doped $Bi_2Sr_2Cu_2O_{8+\delta}$ using extreme ultraviolet (22 eV) probe pulses delivered by a high-harmonic-generation source. This allows us to study the QP relaxation dynamics in selected momentum-space cuts covering the complete Brillouin zone. Our results show that the relaxation of photoexcited QPs is almost momentum-independent taking place on femto- and picosecond time scale.

O 86.9 Thu 17:00 S052

Femtosecond time-resolved photoemission of the photo-induced valence transition in $YbInCu_4$ — •Florian Diekmann, Lars-Philip Oloff, Kerstin Hanff, Michael Bauer, and Kai Rossnagel — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

Below a temperature of 42 K, $YbInCu_4$ displays a first-order isostructural transition from a semimetallic, paramagnetic local-moment phase with an Yb valence of 2.94 to a metallic, non-magnetic, valence-fluctuating heavy-fermion phase with a Yb valence of 2.84 [1]. Here, we use time- and angle-resolved extreme ultraviolet photoemission spectroscopy to directly probe the photo-induced valence transition in the electronic structure relaxation dynamics near the Fermi level on the femtosecond time scale. Temperature- and pump fluence-dependent results are presented and compared to the results of time-resolved reflectivity measurements.
[1] H. Sato *et al.*, Phys. Rev. Lett. **93**, 246404 (2004).

O 86.10 Thu 17:15 S052

Transient band gap enhancement of the photoexcited excitonic insulator phase in quasi-1D Ta_2NiSe_5 — •Selene Mor[1], Marc Herzog[1], Claude Monney[2], Martin Wolf[1], and Julia Staehler[1] — [1]Fritz-Haber-Institut der MPG, Dept. of Phys. Chem., Berlin, Germany — [2]University of Zurich, Physics Dept., Switzerland

Strong electron-hole interaction in small gap semiconductors can lead to spontaneous formation of excitons resulting in an excitonic insulator (EI) phase. Ta_2NiSe_5 (TNS) has been proposed as candidate for such a phase transition (PT) in combination with a structural change at $T_c \approx 328$ K. In order to unveil how the monoclinic/EI phase stabilizes in TNS, we monitor the non-equilibrium dynamics after photoexcitation using time-resolved optical and photoemission spectroscopy. Time-resolved photoemission in the EI phase shows a strong excitation-density-dependent valence band depletion, until absorption saturation is reached at a critical fluence F_{sat}. This is also reflected in a saturation threshold of the overall transient optical response. A coherent phonon at 4 THz, which is specific of the monoclinic phase, persists above F_{sat}, indicative of a hindered photoinduced PT. Time-resolved photoemission below F_{sat} reveals a band gap shrinking due to photoenhanced screening of Coulomb interaction. However, above F_{sat} this process competes with a delayed band gap widening that we attribute to increased excitonic correlations. After $\sim$ 1.5 ps, excess energy is transferred to the lattice and the band gap shrinking is driven quasi-thermally. These complex dynamics support the key role of electron-hole correlations as origin of the EI phase in TNS.

O 86.11 Thu 17:30 S052

Tracing thermal and nonthermal phase transition by pump-probe schemes. Part I: material behavior under irradiation — •Nikita Medvedev[1], Victor Tkachenko[1], and Beata Ziaja[1,2] — [1]CFEL at DESY, Notkestr. 85, Hamburg, Germany — [2]Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Krakow, Poland

We study theoretically effects of thermal and nonthermal phase transitions in semiconductors irradiated with femtosecond laser pulses. Our developed hybrid code XTANT combines: (i) Monte Carlo method tracing highly-excited nonequilibrium electrons; (ii) Boltzmann collision integrals to calculate energy exchange between atoms and low-energy electrons; (iii) tight binding molecular dynamics following atomic motion on the evolving potential energy surface. This combined approach allows to model both, thermal (triggered by heating of atoms via electron-phonon coupling) and nonthermal (triggered by changes of the interatomic potential through electron excitation) phase transition.

In the first part of the report, we present the XTANT model and discuss the behavior of irradiated semiconductors occurring at different timescales. We demonstrate how the electronic kinetics at femtosecond timescales impacts the atomic dynamics. The nonthermal phase transitions occur within a few hundred femtoseconds. Typically at lower excitation doses, thermal heating may lead to structural changes at picoseconds timescales. Examples of irradiated silicon and GaAs will be presented and compared to experiments.

O 86.12 Thu 17:45 S052

Tracing thermal and nonthermal phase transitions in solids with pump-probe scheme. Part II: Response of optical properties — •Victor Tkachenko[1], Nikita Medvedev[1], and Beata Ziaja[1,2] — [1]CFEL at DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Krakow, Poland

Electronic excitation and atomic dynamics after femtosecond laser pulse irradiation affect electronic structure, thus modifying optical properties of irradiated materials. During the transition of the material to non-equilibrium state and its later relaxation to a new equilibrium phase, its optical properties are influenced by both electronic and atomic dynamics. Optical coefficients can be measured in experiments and used as signatures of phase transitions. Pump-probe techniques tracing evolution of optical properties in irradiated material are modelled with our in-house developed XTANT code. As the code is a unified hybrid model that combines Monte-Carlo scheme, temperature equation, molecular dynamics technique and tight-binding formalism, it allows to trace structural transformation of diamond into graphite. The presented method proved to be feasible to evaluate complex dielectric function of the material and hence to calculate reflection, transmission and absorption coefficients of diamond at each stage of the graphitization process. Comparison with experimental data confirms the accuracy of our method.

O 87: Metal Substrates: Structure, Epitaxy and Growth

Time: Thursday 15:00–18:15 Location: S053

O 87.1 Thu 15:00 S053

Zn on Au(111) - growth and alloy formation — •Konstantin M. Schüttler and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Methanol is a promising molecule for chemical energy storage, e.g. by use of H_2 from regenerative sources. Industrially, methanol is synthesized from syngas (CO/H_2) over Cu/ZnO catalysts. The synthesis of “Green Methanol” from CO_2/H_2 as “solar fuel” could make this synthetic fuel even independent of fossil energy carriers. It has recently been demonstrated that under reaction conditions the ZnO support of Cu/ZnO catalysts is partly reduced to Zn, forming a CuZn alloy which is proposed to contain the active site for this reaction. For the hydrogenation of CO_2, Au/ZnO is a highly promising catalyst, and in analogy to Cu/ZnO, reduction of ZnO and formation of bimetallic AuZn surfaces under reaction conditions is plausible.

In order to gain more insight into the formation and nature of active sites, we started to study the formation, structure and chemical properties of bimetallic Zn/Au(111) surfaces as structurally well-defined 2D model catalysts. Here we present first UHV-STM measurements on the growth and (surface) alloy formation of Zn on Au(111). Nucleation and 2D growth of Zn islands seems to start both at the elbow sites of the Au(111) herringbone reconstruction and at step edges. Equally possible, however, is that the observed structures are created by place exchange of Zn atoms into the first layer, which then act as trap sites for Zn and Au adatoms, where the latter result from Zn place exchange. This is tested in ongoing STM experiments.

O 87.2 Thu 15:15 S053

Structural analysis of Pd on W(110) — •Jeannette Kemmer and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We report on a scanning tunneling microscopy (STM) study of the thin-film growth of Palladium (Pd) on W(110). Depending on the Pd thickness various surface superstructures are observed. Sub-monolayer Pd coverages exhibit periodic stripes runing along the [001] direction of the substrate. Their periodicity amounts to (7.3 ± 0.5) nm and does not change significantly up to coverages of 0.88 atomic layers (AL). Additionally, zigzag lines appear in between the straight stripes. Atomically resolved images reveal that these stripes mark transition regions between inequivalent asymmetric Pd adsorption site, i.e. left- and right-shifted relative to the centro-symmetric hollow adsorption site usually found on bcc(110) surfaces. At Pd coverages between 0.93 AL to 1.01 AL the stripe anisotropy along the [001] direction of the substrate decrease. At the same time the stripe periodicity steeply increases, resulting in structural domain sizes up to 100 nm with right- and left-shifted adsorption sites. The second layer starts to grow on step edges and as hexagonal islands with additional stripes on top. The stripes are fully developed when the second layer is completly closed. Island growth starts with the third layer and marks the transition between the bcc crystal structure of the substrate and the fcc crystal structure of the Pd.

Invited Talk O 87.3 Thu 15:30 S053

Heteroatom-doped Molecular Nanostructures on Surfaces — •Sabine Maier — Department of Physics, Friedrich-Alexander University Erlangen-Nürnberg, Germany

The interest in molecular nanostructures on surfaces emerges from their prospective applications in nanoscale electronics, solar cells, energy storage devices, and other fields. Non-covalent intermolecular interactions in self-assemblies facilitate the formation of long-range ordered patterns. In contrast, the on-surface synthesis of covalent molecular structures improves the stability and intermolecular charge transport at the expense of structural control owing to the irreversible nature of the newly formed covalent bonds, which prevents an error correction.

Here, we review recent high-resolution scanning probe microscopy experiments complemented by density functional theory on non-covalent and covalent molecular structures built from carefully designed functionalized triphenylamines. First, hierarchic formation principles of covalently-linked nanoporous networks through surface-assisted Ullmann coupling reactions are shown. Design rules to potentially overcome the lack of long-range order in such networks will be discussed together with their electronic properties and host-guest chemistry. In the second part, electronically decoupled self-assemblies on bulk insulators are presented. We show how intermolecular and molecule-substrate interactions can be tuned by functional groups in order to achieve one-, two-, or three-dimensional assemblies in a controlled way.

O 87.4 Thu 16:00 S053

Atomic diffusion through vacancies as driving mechanism for structure formation of bimetallic surface alloys — •Luis Mancera and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

The local catalytic activity of surface alloys is usually investigated using periodic DFT calculations, and the energetics of the surface structure is based on periodic arrangements. Still, real surface alloys are often far away from having regular atomic distributions. Furthermore, it is not clear whether the resulting structures are governed by thermodynamics, i.e., whether these structures correspond to a minimum of the free energy, or whether their arrangement is a consequence of kinetic hindering that does not allow the system to reach thermal equilibrium. Thus a generalized approach is necessary in order to understand the stability of surface alloys for different mixing ratios of the constituents. Therefore, we investigate the structure formation of surface alloys by generalizing the local description provided by periodic DFT into a kinetic Monte Carlo (kMC) approach that allows to address the temporal evolution of bimetallic structures. As self-diffusion in metals is usually mediated via vacancies, as a first step we concentrate on the determination of transition rates for vacancy diffusion processes taking variations in the local environment into account.

O 87.5 Thu 16:15 S053

The surface reconstruction of Pt(001) revisited — Rene Hammer[1], Oliver Krahn[1], Klaus Meinel[1], and •Wolf Widdra[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck Institut für Mikrostrukturphysik, Halle, Germany

The complex hexagonal reconstruction of the (001) surfaces of platinum and gold is under debate since decades [1,2]. In the present study, we combine SPA-LEED and STM together with LEED simulations based on a Moiré approach to address the Pt(001) reconstruction. Smooth samples annealed at $900°C$ show two domains of a $c(26x128 \pm 10)$ superstructure. The superstructure evolves from a Moiré-like buckling of a quasi-hexagonal top layer (hex). The lattice vectors of the hex are reduced to 0.9606a and 0.9629a with respect to the interatomic distance a of Pt(001). The former runs exactly along [011] or $[01\bar{1}]$ whereas the latter one deviates by 120.08° from that directions. Sample annealing at $1000°C$ stimulates a continuous rotation of the hex where all angles between 0 and $\pm0.8°$ are simultaneously realized. At $1100°C$, the hex resides in fixed rotation angles of $\pm(0.77° \pm 0.01°)$. Sputtering at elevated temperatures lowers the value n of the $c(26x2n)$ superstructure down to 34 and leads to a continuous rotation in the range of $\pm0.8°$. In many aspects, the Pt(001) reconstruction displays a similar behavior as found for Au(001) [2].

[1] P. Havu et al., Phys. Rev. B 82 (2010) 161418(R) and references therein;

[2] R. Hammer et al. Phys. Rev. B 90 (2014) 035446.

O 87.6 Thu 16:30 S053

Mapping the contact formation of a gold tip approaching the Au(111) surface — •Lukas Gerhard[1] and Wulf Wulfhekel[1,2] — [1]Institut für Nanotechnologie (INT), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen — [2]Physikalisches Institut (PI), Karlsruhe Institute of Technology (KIT), 76049 Karlsruhe

The understanding of the interplay between forces, relaxations, and electron transport during formation and breaking of a contact between two metallic electrodes is of fundamental interest for nano-scale electronics. Here we use the gold tip of a low-temperature scanning tunneling microscope (STM) to reproducibly form and break a contact with a reconstructed Au(111) surface without degradation of the electrodes. From a set of about 20.000 individual measurements we mapped the work function, the tip-sample separation at jump into contact, the jump in conductance, and the hysteresis in the approach-retract curve with atomic resolution on an area of 1 x 9 nm ^{2} spanning the 22 x $\sqrt{3}$ unit cell of the reconstruction. The variation of these parameters due to the difference in the local coordination environment is discussed.

O 87.7 Thu 16:45 S053

Epitaxial growth of tin(IV)-phthalocyanine-dichloride on Ag(111) — •Christian Zwick[1], Yui Ioka[2], Roman Forker[1], Satoshi Kera[2,3], and Torsten Fritz[1] — [1]Institute of Solid State Physics , Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Graduate School of Advanced Integration Science, Chiba University, Yayoi-cho, Inage-ku, Chiba 2638522, Japan — [3]Institute for Molecular Science, Myodaiji, Okazaki 4448585, Japan

The peculiarities of the tetrahedron-like organic dye molecule tin(IV)-phthalocyanine-dichloride ($SnCl_2Pc$) originate from its functionalization with chlorine atoms above and below the central tin atom. These are expected to have a crucial impact on interface formation by virtue of their role as spacer groups and also due to the altered chemical reactivity compared to chlorine-free phthalocyanines. We report on the coverage-dependent growth of $SnCl_2Pc$ on Ag(111). The thin films were characterized optically by in situ differential reflectance spectroscopy (DRS) and structurally by combined scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) measurements. Depending on the effective layer thickness we observe distinct phases of highly ordered flat-lying $SnCl_2Pc$ molecules, leading to a bilayer structure as a precursor for a bulk-like crystal growth. For each of the subsequently observed structural phases, distinct optical properties can be assigned, allowing to qualitatively judge possible interactions with the surface and between stacked molecular layers in addition to the characterization of the structural reordering processes.

O 87.8 Thu 17:00 S053

On the adsorption behavior of a porphyrin on different Cu surfaces: A comparative scanning tunneling microscopy study — •Michael Lepper, Liang Zhang, Michael Stark, Hans-Peter Steinrück, and Hubertus Marbach — Physikalische Chemie II and Interdisciplinary Center for Molecular Materials

(ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

Self-assembly of functional molecular building blocks on well-defined surfaces is a promising approach for the bottom-up fabrication of two-dimensional nanostructures with outstanding properties. In this respect, porphyrins are particularly attractive due to their distinct chemical and physical properties. In this study, we compare the adsorption of 2H-5,10,15,20-Tetrakis-(3,5-di-tert-butyl)-phenylporphyrin (2HTTBPP) on different substrates, i.e., Cu(110) and Cu(110)-(2x1)O, under ultra-high vacuum conditions by scanning tunneling microscopy. At room temperature, supramolecular arrangements are observed for 2HTTBPP on Cu(110)-(2x1)O, while on Cu(110) individual molecules in a disordered layer are found. Interestingly, the intramolecular conformations on the two substrates are quite different. The corresponding findings are interpreted by accounting for specific molecule-molecule and molecule-substrate interactions. In addition, the so-called self-metalation of 2HTTBPP with Cu atoms will be reported and discussed. Supported by the DFG through FOR 1878 (funCOS) and the AvH Stiftung.

O 87.9 Thu 17:15 S053

From Porphyrins to Pyrphyrins: Adsorption and Metalation on Au(111) — •Gerson Mette[1], Denys Sutter[1], Yeliz Gurdal[2], Stephan Schnidrig[2], Benjamin Probst[2], Marcella Iannuzzi[2], Jürg Hutter[2], Roger Alberto[2], and Jürg Osterwalder[1] — [1]Physik-Institut, Universität Zürich, CH-8057 Zürich — [2]Institut für Chemie, Universität Zürich, CH-8057 Zürich

Pyrphyrin, a tetradentate bipyridine based macrocycle, represents an interesting but widely unexplored molecular ligand. It shares some similarities with the far better known porphyrins, but it is constituted by pyridyl subunits instead of pyrrols. A high stability of pyrphyrin and its corresponding complexes is suggested. Metal complexes based on pyrphyrin ligands have recently shown promise as water reduction catalysts in homogeneous photochemical water splitting reactions [1].

In this study, we examined the adsorption and metalation of pyrphyrin on a single crystalline surface by means of low-energy electron diffraction (LEED), scanning tunneling microscopy (STM), x-ray photoelectron spectroscopy (XPS) and density functional theory (DFT). Pyrphyrin coverages of approximately one monolayer and less were obtained by sublimation of the molecules on a Au(111) surface at room-temperature. Cobalt deposition and subsequent annealing led to the formation of Co-ligated pyrphyrin molecules. An intermediate state of the metalation reaction was observed and the reaction steps for the Co metalation of pyrphyrin molecules on Au(111) were established.

[1] E. Joliat et al., (in preparation).

O 87.10 Thu 17:30 S053

Structure and morphology of sulfur-terminated Si(111) — •Lars Buss, Thomas Schmidt, and Jens Falta — Universität Bremen, Bremen, Germany

The preparation of sulfur-terminated Si(111)-surfaces aims at the functionalization and passivation of the surface as a template for the growth of layered materials thin films, as the sulfur-termination prevents strong chemical bonding between the substrate and the adsorbate. Therefore the surface-reconstruction and the morphology of the sulfur-terminated Si(111)-surface have been examined with both SPA-LEED and STM. In a small temperature range, a phase transition from (7×7) to a reconstruction, previously reported as (4×4) by Metzner et al. (Surf. Sci. **377** (1997) 71), was found. Our analysis, however, reveals that this reconstruction is actually a $\left(\begin{smallmatrix}2&0\\1&2\end{smallmatrix}\right)$-reconstruction, which occures in three rotational domains on the surface. Furthermore we observe that the surface is etched upon prolonged exposure to the sulfur-flux.

O 87.11 Thu 17:45 S053

Decay of isolated Hills and Saddles on Si(001) studied by LEEM — •Pierre Kirschbaum[1], Lothar Brendel[1], Kelly R. Roos[2], Michael Horn-von Hoegen[1], and Frank-J. Meyer zu Heringdorf[1] — [1]Faculty of Physics and Center of Nanointegration (CeNIDE), University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg — [2]Present Adress: Faculty of Engineering and Physics, Bradley University, Preoria, IL 61625

Dark field low energy electron microscopy is used to study the high temperature decay of isolated hills and saddle points on Si(001). We find different temperature dependent decay rates for the top of the hill compared to a saddle point with low step density that is present in the vicinity of the hill. The decay rate of the hill is always higher than the decay rate at the saddle. The two rates converge with increasing temperature and become equal at temperatures above 1060°C. We also report an alternating fast and slow decay rate for the layer-by-layer decay of the hills. This surprising finding is independent of temperature and is explained by macroscopic strain in the sample. In-situ deposition of Au on the Si(001) surface increases the decay rates of the hill and saddle by more than a factor of ten.

O 87.12 Thu 18:00 S053

Growth, morphology, and stoichiometry of cobalt germanide islands on Ge(001) — •Moritz Ewert[1], Thomas Schmidt[1], Inga Heidmann[1], Jan Ingo Flege[1], Tomasz Grzela[2], Michael Foerster[3], Lucia Aballe[3], Thomas Schroeder[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Leibniz Institute for Innovative Microelectronics (IHP), Frankfurt (Oder), Germany — [3]ALBA CELLS, Barcelona, Spain

In today's silicon technology, the integration of germanium structures is one of the most promising routes to improve the performance of CMOS devices. One of the challenges is the fabrication of low-resistance metal/Ge contacts. As metallization contact materials, Co germanides and Ni germanides are regarded to have the best perspective.

We have investigated the growth of Co germanide on Ge(001) by Co metal deposition using low-energy electron microscopy and microdiffraction as well as x-ray absorption photoemissionmicroscopy (XAS). Both for room temperature (RT) deposition followed by thermal annealing as well as for metal deposition at elevated temperatures, we observe the formation of Co germanide 3D islands. Extremely anisotropic, needle-like 3D islands extending in {110} directions coexist with rather compact ones. XAS measurements at the Co L absorption edge show that for deposition at room temperature, metallic Co is present on the surface that reacts with the Ge during subsequent thermal annealing. The Co germanide forms 3D Volmer-Weber islands. Interestingly, local XAS reveals that different island morphologies are related to different germanide stoichiometries.

O 88: Frontiers of Electronic Structure Theory: Focus on Topology and Transport V

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

O 88.1 Thu 15:00 H24

Zero-point renormalization of the electronic structure: trends across chemical and structural space — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

The importance of the renormalization of the electronic structure due to the zero-point nuclear motion (ZPR) has been discussed since long [1,2], but only recent advances in the first-principles treatment of electron-phonon coupling (EPC) enabled an accurate assessment of this effect for simple, prototypical materials, e.g., diamond [3] and Si [4]. However, it is largely unknown how chemical and structural properties affect the ZPR. To shed light on this question, we compute the EPC and ZPR for the octet binaries in both the zincblende and NaCl structure. Computationally, this is achieved by exploiting our recent implementation of density-functional perturbation theory in real-space, which provides considerable computational advantages with respect to numerical costs, parallelization, and especially scalability with respect to the number of atoms. We demonstrate the validity of our implementation by comparing with existing studies and finite difference results, investigate the trends across chemical/structural space, and critically discuss the role of the exchange-correlation functional.

[1] P. B. Allen and V. Heine, J. Phys. C **9**, 2305 (1976).
[2] M. Cardona, Solid State Commun. **133**,3 (2005).
[3] F. Giustino,*et.al.* Phys. Rev. Lett. **105**, 265501 (2010).
[4] S. Poncé, *et.al.* J. Chem. Phys. **143**, 102813 (2015).

O 88.2 Thu 15:15 H24

All-Electron Many-Body Approach to X-Ray Absorption Spectroscopy — •Christian Vorwerk, Caterina Cocchi, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

We present an all-electron approach of the many-body perturbation theory to describe X-ray absorption spectroscopy (XAS) in solid-state materials. In this formalism, the electron-hole interaction is explicitely included by solving the Bethe-Salpeter equation. A fully relativistic description of core states, as implemented in the all-electron full-potential code `exciting`[1], enables the explicit treatment of the effects of spin-orbit coupling in the spectra. We investigate the XAS for prototypical systems, such as TiO$_2$ and MgO, considering excitations from oxygen K and metal L edges. Our results, in good agreement with experiments, allow us to gain insight into the nature of the core-level excitations of these materials.

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

O 88.3 Thu 15:30 H24

Cohesive properties from all-electron RPA total energies — •Markus Betzinger[1], Christoph Friedrich[1], Andreas Görling[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

We present an all-electron implementation of the RPA total energy within the full-potential linearized augmented plane-wave (FLAPW) method. An incomplete basis-set correction (IBC) [1] is employed to improve the convergence of the total energy with respect to the basis-set and the number of unoccupied states. To some extent the IBC incorporates an infinite number of bands and enables a virtually exact treatment of the core electrons.

We demonstrate that the core electrons give rise to a sizeable contribution to the RPA total energy. Their individual contribution is comparable to that of the valence electrons. All-electron RPA lattice constants and bulk moduli are shown for a set of prototype materials and compared to experimental results. An excellent agreement with experiment is observed.

[1] M. Betzinger *et al.*, Phys. Rev. B (accepted, 2015); **88**, 075130 (2013); **85**, 245124 (2012).

O 88.4 Thu 15:45 H24

Explicitly correlated self consistent field theory — •Christian Lasar and Thorsten Klüner — Universität Oldenburg

Explicitly correlated correlation methods are an interesting field of current research since they are able to drastically improve the otherwise slow basis set convergence of conventional correlation methods. Therefore, chemical accuracy can be achieved with rather small basis sets.[1] The new correlation method presented in this contribution has already been developed for two-electron systems a long time ago[2]. We present the generalization of this ansatz to N-electron systems.

The basic idea is to augment a single slater-determinant with an explicitly correlated prefactor which then takes care of the correlation effects and the basis set convergence. Another interpretation of this ansatz would be a contracted CISD with orbital optimization in a complete basis set. The contraction is achieved by the explicitly correlated prefactor whose choice therefore defines the possible accuracy of the method. In principle, the generalization to any pair method i.e. CCSD and MP2 will be possible.

The big advantage of this kind of ansatz for the wave function is the drastic reduction of matrix elements needed for the optimization of the wave function. As a result, the presented method will be applicable to large molecules.

[1] Chem. Rev. 112, p. 4 (2012) [2] J. Chem. Phys. 99, p. 8830 (1993)

O 88.5 Thu 16:00 H24

Representing energy landscapes by combining neural networks and the empirical valence bond method — •Sinja Klees[1], Ramona Ufer[2], Volodymyr Sergiievskyi[2], Eckhard Spohr[2], and Jörg Behler[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, D-45141 Essen, Germany

In recent years, artificial neural networks (NNs) have become a powerful method to develop reactive interatomic potentials for large systems. However, the construction of NN potentials can become computationally very demanding due to the high dimensionality of the configuration space, which needs to be mapped by reference electronic structure calculations. Combining NN potentials with the empirical valence bond (EVB) method offers a promising approach to derive the potential energy of complex systems with substantially reduced effort, since the size of the reference structures can be strongly decreased. Preliminary results will be discussed and compared to density functional theory data.

O 88.6 Thu 16:15 H24

CELL: a python package for cluster expansions with large parent cells — •Santiago Rigamonti[1], Maria Troppenz[1], Christopher Sutton[2], Luca M. Ghiringhelli[2], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft

The discovery of new materials for applications in areas such as energy harvesting, relies more and more on the accurate theoretical description of complex structures with large unit cells. The properties of interest are often tuned by substitutional dopants. Due to the vast configurational dopant space, a wide-spread approach is the cluster expansion (CE) technique. Most available CE codes are designed for alloys based on small parent cells, with usually 1 to 4 atoms. For the many important materials with much larger parent cells such approaches can't be applied. We devise an iterative scheme, based on efficient samplings of the configurational space, avoiding full structure enumerations. CELL consists of several modules that can be used independently, enabling to design CEs for specific purposes. Various CE schemes are available, offering ℓ_2 and ℓ_1 norms as penalization terms and different cross-validation strategies. Methods such as LASSO and split Bregman iteration are available for dealing with the ℓ_1 norm (compressive sensing). Access to finite-temperature properties and the characterization of phase transitions is possible through the Wang-Landau and diffusive nested sampling modules. Examples are presented for type-I thermoelectric clathrates, with 46 sites in the parent cell.

O 88.7 Thu 16:30 H24

Structural and electronic properties of the thermoelectric clathrates $\mathbf{Ba_8Al_xSi_{46-x}}$ and $\mathbf{Sr_8Al_xSi_{46-x}}$ — •Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

Clathrate compounds are promising candidates for high-efficiency thermoelectric applications. Their cage-like structure containing guest atoms allows for exploiting the idea of the phonon-glass electron-crystal and reaching a large figure of merit. We study $\mathrm{Ba_8Al_xSi_{46-x}}$ and $\mathrm{Sr_8Al_xSi_{46-x}}$ ($6 \leq \mathrm{x} \leq 16$), where optimal electronic properties are expected close to the Zintl composition ($\mathrm{x} = 16$). Cluster expansions on various quantities are performed, thus having access to ground-state as well as finite-temperature properties. A linear increase of the lattice constant with the number of Al substituents is obtained (0.019 Å per Al addition) confirming experimental observations (0.02 Å). The calculated bond distances between high-symmetry sites agree well with experiment for the full compositional range [1,2]. We find a close correlation between bond distances and fractional Al occupancies. This helps improving models used by experimentalists to estimate fractional occupancies. The substitutional configurations present an order-disorder transition around $600-900\,\mathrm{K}$, which is further analyzed applying the Wang-Landau method. An important finding is the semiconducting behavior of the low-temperature ordered phase at the Zintl composition, which points out the technological relevance of these compounds.

[1] J. H. Roudebush *et al.*; *Inorg. Chem.* **51**, 4161 (2012)

[2] M. Bobnar *et al.*; *Dalton Trans.* **44**, 12680 (2015)

O 88.8 Thu 16:45 H24

***Ab-initio* calculation of Raman spectra of graphene-based materials** — •Albin Hertrich, Caterina Cocchi, Pasquale Pavone, and Claudia Draxl — Department of Physics, Humboldt-Universität zu Berlin, Germany

Raman scattering is an important non-destructive method for characterizing carbon-based materials. The main features of experimental Raman spectra of pristine graphene and graphite are the first-order G-band at ≈1580 cm^{-1} and the dispersive second-order 2D-band at ≈2700 cm^{-1}. We calculate first- and second-order Raman spectra fully *ab-initio* using the full-potential all-electron DFT package `exciting` [1], which allows for the calculation of both phonon dispersion, within the frozen-phonon approximation, and frequency-dependent dielectric tensors, from time-dependent DFT and the Bethe-

Salpeter equation. In our approach [2], we expand the dielectric tensor with respect to the phonon normal coordinates. By taking its derivatives and by computing vibrational matrix elements, we calculate Raman scattering intensities. Applying this scheme to monolayer graphene, bilayer graphene, and graphite, we obtain the G-band in good agreement with experiment [3]. Furthermore, we explore the influence of both the stacking sequence and the laser energy on the 2D-band.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] C. Ambrosch-Draxl *et al.*, Phys. Rev. B **65**, 064501 (2002).
[3] A. C. Ferrari *et al.*, Phys. Rev. Lett. **97**, 187401 (2006).

O 88.9 Thu 17:00 H24

Exciton dispersion in layered and 2D systems — •Francesco Sottile[1,2], Giorgia Fugallo[1,2], Pierluigi Cudazzo[1,2], and Matteo Gatti[1,2,3] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-IRAMIS, Université Paris-Saclay, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility — [3]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, Boîte Postale 48, F-91192 Gif-sur-Yvette, France

The study of the exciton dispersion is of paramount importance for all applications involving light harvesting, beside providing fundamental knowledge about exciton mobility and migration. Using state-of-the-art ab initio many-body approach, like the Bethe-Salpeter equation [1], we present a first principle study of exciton dispersions in layered materials and 2D systems. Results for the former systems (on the prototypical hBN and MoS2) have been recently confirmed by experiments carried out at the Synchrotron ESRF [2]. For the latter (2D) systems we investigate exciton dispersion in graphane and hBN. From our results we provide a general picture of the mechanisms governing the dispersion of neutral excitations in 2D systems, and of the role played by the confinement of the electronic charge in setting the exciton binding energy. In particular we found that due to the strongly reduced screening of the Coulomb interaction in low- dimensional materials, the binding energy of both Wannier and Frenkel excitons in the optical spectra is large and comparable in size[3]. [1] M. Gatti et al., Phys. Rev. B 88, 155113 (2013) [2] G. Fugallo et al. Phys. Rev. B 92, 165122 (2015) [3] P. Cudazzo et al. submitted to Phys. Rev. Lett.

O 88.10 Thu 17:15 H24

Electronic structure of selected superheavy elements (Z>104) — •Hana Cencarikova[1] and Dominik Legut[2] — [1]Institute of Experimental Physics, SAS, Kosice, Slovakia — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

The electronic structure of selected super-heavy elements (Z>104) have been determined from the first-principle calculations based on the density functional method. To determine the ground-state structure we have calculated number of basic phases including the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures. Our results were obtained using local density approximation for the exchange and correlation effects and without and with the spin-orbit interaction for the band states. The analysis has been focused on the determination of the electronic density of states, electronic band structure dispersion relation, mechanical properties (elastic constants) and selected thermodynamical properties.

O 88.11 Thu 17:30 H24

Layer-resolved calculated vibrations at gold surfaces — •Andrei Postnikov[1] and Kamil Moldosanov[2] — [1]Université de Lorraine, LCP-A2MC, Metz, France — [2]Kyrgyz-Russian Slavic University, Bishkek, Kyrgyzstan

Vibration modes at (001), (011) and (111) surface of gold are calculated from first principles, using the Siesta method [1] and the frozen phonon approach. Calculations are done on thick slabs of moderate lateral size – (2×2) for (001), (2×3) for (011), (3×3) for (111). This allows to resolve the vibration patterns layer by layer into the depth, in dependence on the in-plane wavevector component, and discriminating the polarisation of vibration modes. One notes the softening of modes at the surface, and an appearance of specifically surfacial modes. The bulk behaviour is largely recovered from the 5th or 6th layer downwards.

This study was driven by an intention to grasp the properties of longitudinal acoustic modes propagating at some depth under the surface of gold nanoparticles, which were an important element of our recent work related to the mechanism of radiofrequency absorption and hence resulting heating of nanoparticles of $\gtrsim 5$ nm size [2]. Since it is difficult to meaningfully incorporate the diversity of the nanoparticles' shapes in a practical calculation, the vibrations beneath the most common facets occurring at the nanoparticles' surface were studied instead.

1. The Siesta method, `http://departments.icmab.es/leem/siesta/` .
2. A. Postnikov and K. Moldosanov, `http://arxiv.org/abs/1508.00735` .

O 88.12 Thu 17:45 H24

Electronic structure, mechanical and thermodynamic properties of Actinium from first-principles — •Zuzana Grosmanova[1] and Dominik Legut[2] — [1]Nanotechnology, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

In this work, the mechanical (elastic constants) and thermodynamic properties of actinium were investigated using first-principle calculations. Our results were obtained using density functional theory employing local density and general gradient approximation for the electronic exchange-correlation effects and including the spin-orbit interaction for the band states. The ground-state structure were determined among simple phases like the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures.

O 88.13 Thu 18:00 H24

Interaction of Tritium and Chlorine 36 with defects in Graphite: Insights from Theory — •Christoph Lechner[1], Philippe Baranek[1], and Holger Vach[2] — [1]EDF Lab Les Renardières, Avenue des Renardieres, F-77818 Moret-sur-Loing Cedex, France — [2]CNRS-LPICM, Ecole Polytechnique, F-91128 Palaiseau Cedex, France

In order to optimize the waste management of nuclear graphite used in power plants, it is important to understand the properties of the activated impurities it contains, such as tritium and chlorine 36. Therefore, a computational study of the interaction of tritium and chlorine 36 with defects in graphite has been achieved at the density functional theory (DFT) level by using the functionals PBE and PBE0 with Grimme's D3 dispersion correction. The physisorption and chemisorption of atomic and molecular hydrogen or chlorine on graphite surfaces, (001), (100), and (110) with or without mono- and divacancies, have been investigated. The stabilities of the formed complexes are interpreted in terms of the formation energy. To obtain insight into the nature of the bonding a population analysis of the systems has been performed. While the bonding of hydrogen is mostly covalent for chemisorption and van der Waals for physisorption, the behavior of chlorine is much more complex. Depending on the defect site, both, dominantly covalent and dominantly charge transfer bonding, is observed. Raman spectra for selected structures have been investigated, in order to evaluate, if the experimentally observed defect bands can be reproduced.

O 89: Oxides and Insulator Surfaces II

Time: Thursday 15:00–18:30 Location: H4

O 89.1 Thu 15:00 H4

Iron-Silicate films on Ru(0001) — •Gina Peschel, Hagen W. Klemm, Alexander B. Fuhrich, Mauricio Prieto, Dietrich Menzel, Thomas Schmidt, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland

Zeolites offer strong catalytic activity and are already widely used in industry as desiccant, detergent or as molecular sieves. Iron-silicate could be seen as a model system, offering the possibility to understand structure and reactivity correlations and functionalize these materials even more. Our investigation addresses the growth and structure of ultrathin iron-silicate films on a Ru(0001) substrate with the methods of LEEM, LEED, XPS and XPEEM.

Our studies reveal the formation of co-existing structural domains. XPEEM results indicate that one kind of domain contains iron and silicon while the other domain type contains only silicon. The overall

LEED pattern consists of a $(\sqrt{3} \times \sqrt{3})$ R30° pattern with Moiré spots, superimposed with a (2×2) structure, which could be assigned to the individual domains, respectively. Including additional XPS results we suggest a model for the iron-silicate consisting of a silica layer bound to a complete FeO layer on the Ru-support.

O 89.2 Thu 15:15 H4

AFM investigation on CaF2(111) with atomically characterized tips — •Alexander Liebig, Daniel Meuer, Angelo Peronio, and Franz Josef Giessibl — Universität Regensburg, Germany

Contrast formation in atomic force microscopy (AFM) images of ionic systems is often dominated by the electrostatic interaction between the ions of the sample and the tip apex. Thus, the chemical identity of the latter determines the contrast pattern, as e.g. shown for NaCl bilayers on the Cu(111) surface by Gross et al. [1]. To optimize atomic contrast in AFM experiments, the tip is usually poked slightly into the surface, ending up with picking up a cluster of sample atoms by the tip. The tip termination is thus uncharacterized, hindering the discrimination of the different species of atoms in the AFM images. In this work, the CaF2(111) surface is studied by AFM measurements. In contrast to ionic crystals of the rock salt structure, the surface ions of CaF2(111) are all charged negatively [2] and the contrast of the image allows to determine the tip polarity [2,3]. Similar to previous experiments on Cu2N [4], we use tips that are characterized at the atomic level using COFI [5], where an adsorbed CO molecule is used to image the tip apex. Our goal is to characterize the imaging mechanisms and the electrostatics of our different tips on the CaF2(111) surface.

References: [1]: L. Gross et al., Phys. Rev. B 90, 155455 (2014). [2]: A. Foster et al., Phys. Rev. Lett. 86, 2373 (2001). [3]: F. J. Giessibl, M. Reichling, Nanotechnology 16, 118 (2005). [4]: M. Schneiderbauer et al., Phys. Rev. Lett. 112, 166102 (2014). [5]: J. Welker et al., ACS Nano 7, 7377 (2013).

O 89.3 Thu 15:30 H4

(100)-oriented CeO_2 Nanoislands: Structure and Polarity Compensation — •Niklas Nilius[1], Yi Pan[2], Hans-Joachim Freund[2], Claudine Noguera[3], and Jacek Goniakowski[3] — [1]Carl von Ossietzky Universität Oldenburg, Institut für Physik, D-26111 Oldenburg, Germany — [2]FHI-Berlin, Fradayweg 14-16, D-14195 — [3]CNRS-Sorbonne Universités, UPMC Univ. Paris 06, UMR 7588, INSP, F-75005 Paris, France

Compact CeO_2(111) films grown on Ru(0001) can be transformed into well-shaped nanoparticles by annealing them in an oxygen-poor environment. With increasing temperature, the particles undergo a shape evolution that finally leads to crystallites exposing wide (100) facets. The atomic structure of the (100) termination has been determined with a combination of high-resolution scanning tunneling microscopy and density functional theory. Two surface reconstructions are identified, composed either of CeO_4 nano-pyramids in a (2×2) arrangement or oxygen adatoms forming a c(2×2) super-structure. Both terminations enable full compensation of the polar dipole intrinsic to CeO_2(100), but also reflect a gradual reduction of the oxide that proceeds from the surface. Our study provides insights into the rarely explored (100) termination of ceria, which represents a good model system for structurally open and polar oxide surfaces.

O 89.4 Thu 15:45 H4

Thin Silica films on Ru(0001) — •Hagen William Klemm, Gina Peschel, Alexander Benedikt Fuhrich, Mauricio Prieto, Dietrich Menzel, Thomas Schmidt, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4, 14195 Berlin, Germany

Ultrathin SiO_2 and metal doped silicate layers on Ru(0001) offer various possibilities as model systems for understanding the relationship between structure and reactivity of very complex material systems like Zeolites. With the aberration corrected spectro-microscope SMART at the synchrotron light source BESSY-II in Berlin, allowing high-resolution XPEEM, μXPS, valence band mapping, μ-LEED and LEEM, preparation conditions and their influence on the Silica layers were studied *in situ* at the mesoscopic scale. The deposited amount of Silicon and the oxidation conditions strongly influence the crystallographic and electronic structure of these Silica films. SiO2 bilayer films are of special interest, because they are only Van de Waals like bound to the Ru(0001) substrate and therefore lift off the support. Under special preparation conditions an oxidation front, followed by an oxygen intercalation could be observed.

Invited Talk O 89.5 Thu 16:00 H4

The growth and decay of oxide quasicrystals — •Stefan Förster[1], Jan Ingo Flege[2], Eva Maria Zollner[1], Florian Schumann[1], Klaus Meinel[1], Jens Falta[2], and Wolf Widdra[1,3] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Institute of Solid State Physics, University of Bremen, Bremen, Germany — [3]Max Planck Institute of Microstructure Physics, Halle, Germany

Two-dimensional materials have recently pioneered a new field of materials science. Their peculiar properties are often related to their lower dimensional periodic structure. A new member in this class of materials are two-dimensional oxide quasicrystals (OQC)[1]. Here I will present the first in-situ high-temperature characterization of the $BaTiO_3$-derived OQC. This OQC develops in a 2D wetting layer spreading from 3D $BaTiO_3$ islands on Pt(111) and exhibits a sharp twelvefold diffraction pattern [1]. The structure formation process includes the growth of an amorphous wetting layer which can either develop further into the OQC or into long-range ordered periodic structures, the so-called approximants. Insights into this process are derived from combining the findings of scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) measurement with in-situ low-energy electron microscopy (LEEM) studies. Besides the details of the quasicrystalline growth process, the in-situ LEEM and μ-LEED studies reveal also the high-temperature stability of this new phase.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, Nature 502, 215 (2013).

O 89.6 Thu 16:30 H4

Another 2-dimensional oxide quasicrystal: Strontium titanate on Pt(111) — •Sebastian Schenk[1], René Hammer[1], Florian Schumann[1], Stefan Förster[1], Klaus Meinel[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

Recently the formation of a $BaTiO_3$-derived 2-dimensional oxide quasicrystal (OQC) with 12-fold diffraction symmetry has been discovered on Pt(111) substrates [1]. Following an analogous preparation procedure, we show that $SrTiO_3$ on Pt(111) develops an OQC as well. First, a closed $SrTiO_3$ film on Pt(111) has been prepared using MBE. The stoichiometry and structure of the film has been analyzed by means of AES and SPA-LEED. Annealing the film in an O_2 atmosphere yields the formation of 3-dimensional $SrTiO_3$ islands with bare Pt(111) in between. Annealing in UHV causes a rewetting on the Pt(111) via surface diffusion of $SrTiO_3$ from the islands. SPA-LEED and STM reveal that at temperatures around 700°C an OQC is formed in the rewetting layer. The $SrTiO_3$ derived OQC is composed by quadratic, triangular, and rhombic elements of equal side length of about 0.6 nm. They form an aperiodic structure, which displays a well-ordered 12-fold diffraction pattern. Our results suggest that OQC formation is a general process of oxide perovskites on suitable substrates.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, Nature 502 (2013) 215.

O 89.7 Thu 16:45 H4

Software-based analysis of aperiodic structures of quasicrystals — •Berit Schreck[1], Stefan Förster[1], René Hammer[1], Klaus Meinel[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The discovery of a novel class of oxide quasicrystals (OQC) leads to a new field in surface and material science research. $BaTiO_3$ develops a 2D structure of twelve-fold rotational symmetry when prepared as thin film on Pt(111) [1]. In order to determine the atomic structure and the statistics of the tiling, a software based approach for the drift correction and the extraction of atomic coordinates from atomically resolved STM images has been developed. The OQC structure is composed by an aperiodic arrangement of triangular, quadratic, and rhombic building blocks, comparable to the Stampfli-Gähler-Tiling [2]. Angles, edge lengths, and frequency of occurre of the OQC tiling elements have been extracted and will be compared with the theoretical model.

[1] Förster, S. et al., Nature 502, 215 (2013). [2] Gähler, F. in Quasicrystalline Materials, Ch. Janot and J.M. Dubois (eds.), World Scientific (1988).

O 89.8 Thu 17:00 H4

Transition metal-oxide hybrid chain structures on Ir(100) - a general trend? — •Pascal Ferstl[1], Florian Mittendorfer[2], Christopher Sobel[1], Matthias Gubo[1], Klaus Heinz[1], Josef Redinger[2], M.Alexander Schneider[1], and Lutz Hammer[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg — [2]Institut für Angewandte Physik & CMS, TU Wien

We show that the oxidation of a 1/3 monolayer of different transition metals (Mn, Co, Fe and Ni) on the Ir(100) surface leads to the formation of a surface oxide of nearly the same crystallographic structure. All of the metals (Me) form quasi-one-dimensional chains of MeO_2 stoichiometry and grow exclusively with threefold lateral spacing on the plain Ir(100) terraces forming an almost defect-free 3×1 superstructure. This allows for a quantitative determination of the crystallographic structure of the chains by means of full dynamical LEED-IV analyses which resulted in Pendry R-factor values around 0.11 for all investigated systems. The best fit structures were independently confirmed by DFT calculations. The MeO_2 stripes only bind via the oxygen atoms to the substrate, while the central mono-atomic metal wire is decoupled from its Ir neighbours. The only notable difference between the various metal-oxide hybride structures is the buckling of the Me atom with respect to the first Ir layer that varies between 1.1 and 0.7 Å.

O 89.9 Thu 17:15 H4

Growth and morphological characterization of thin vanadium dioxide films — •Mirco Schulz, Jon-Olaf Krisponeit, Jan Ingo Flege, and Jens Falta — Universität Bremen, Bremen, Germany

Vanadium dioxide exhibits a metal-insulator transition near room temperature, comprising a rich phenomenology that is still not fully understood. Close to the transition, the system responds sensitively to uniaxial substrate-induced stress, resulting in a wide variation of the transition temperature. In this contribution, thin VO_2 films were grown on $TiO_2(001)$ and $TiO_2(110)$ substrates by molecular beam epitaxy. Two different growth methods were used: first, vanadium evaporation under O_2 ambient and, second, cyclic vanadium deposition and post-annealing in O_2, following an approach by J. W. Tashman et al. [1]. For both methods the prevalence of the V^{4+} oxidation state was confirmed by x-ray photoelectron spectroscopy. The surface structure was analyzed with low energy electron diffraction, indicating an epitaxial growth on the substrate and good crystallinity of the films. While scanning tunneling microscopy revealed continuous films of VO_2 on both substrates, we found faceting in the case of (110) substrate orientation, but terraces on (001) substrates.

[1] J. W. Tashman et al., Appl. Phys. Lett. **104**, 063104 (2014).

O 89.10 Thu 17:30 H4

SMSI effect of a non-reducible oxide: ZrO_2/metal inverse model catalysts — •Michael Schmid, Peter Lackner, Joong-Il J. Choi, and Ulrike Diebold — Institut f. Angewandte Physik, TU Wien, Vienna, Austria

Many oxide-supported metal catalysts exhibit the so-called SMSI (strong metal-support interaction) effect, where the metal gets overgrown by an ultrathin oxide layer under reducing conditions [1,2]. This effect is usually limited to reducible oxides, and the ultrathin oxide is substoichiometric. We have deposited few-layer ZrO_2 films on Pt and Rh(111) surfaces and find dewetting upon annealing to high temperatures in oxygen, i.e., between the oxide islands the bare metal surface gets uncovered. Annealing in ultrahigh vacuum instead leads to a structure akin to Stranski-Krastanov growth, i.e., oxide islands with the metal in between covered by an ultrathin oxide, as in SMSI systems. We identify this ultrathin oxide as an essentially stoichiometric ZrO_2 trilayer [3], thus the reason for the SMSI effect observed must be different from the usual variation of oxide stoichiometry. We propose a new mechanism for the SMSI effect, which is alloying between Zr and the metal, modifying the metal-oxide bonding.

[1] Tauster, Fung, Baker, Horsley, Science 211, 1121 (1981).
[2] Dulub, Hebenstreit, Diebold, Phys. Rev. Lett. 84, 3646 (2000).
[3] Antlanger et al., Phys. Rev. B 86, 035451 (2012).

O 89.11 Thu 17:45 H4

Thermal Reduction of Au(111)-Supported Cuprous Oxide Films — •Hanna Fedderwitz[1], Claudine Noguera[2], Jacek Goniakowski[2], and Niklas Nilius[1] — [1]Carl von Ossietzky Universität Oldenburg, Institut für Physik, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne Universités, UPMC Univ. Paris 06, UMR 7588, INSP, F-75005 Paris, France

Thin Cu_2O films with stoichiometric (111)-termination and a band gap of 2.0 eV are prepared by reactive Cu deposition on Au(111) surfaces. Annealing to temperatures above 700 K, both in vacuum and $5 * 10^{-6}$ mbar of oxygen, results in a gradual reduction of the oxide, as monitored by XPS and STM. The reduction process starts off with the appearance of single Cu atoms and small clusters at distinct sites of the $Cu_2O(111)$ lattice. At higher temperature, metallic Cu patches develop at the surface, clearly distinguishable from the oxide domains via their deviating atomic and electronic structure. Simultaneously, bare Au(111) regions emerge, which coexist with the Cu and Cu_2O domains and continuously increase in size at higher temperature. Additional insight into the Cu_2O to Cu transition comes from characteristic changes of the Cu LVV Auger lines, as probed with XPS. The observed reduction behavior of thin-film Cu_2O is rationalized with the help of stability diagrams derived from DFT*based ab-initio thermodynamics.

O 89.12 Thu 18:00 H4

ALD growth of Al_2O_3 on Stepped Surface of HOPG and Ag-HOPG — •Zied Rouissi[1], Karsten Henkel[1], Massimo Tallarida[2], and Dieter Schmeisser[1] — [1]Brandenburg University of Technology Cottbus-Senftenberg — [2]ALBA Synchrotron, 08290 Cerdanyola del Vallès, Barcelona, Spain

Atomic Layer Deposition (ALD) is an excellent deposition technique to grow thin film with high homogeneity coverage on ideal surfaces. Here we are interested in the growth properties on non-ideal (stepped, inert) surfaces. Using STM we studied the growth of Al_2O_3 by ALD on stepped surface of HOPG and silver covered HOPG (Ag-HOPG). The HOPG sample was cleaved to and then cleaned by N2 in vacuum. We obtain regular steps with terrace widths of 50nm * 500nm. Ag was deposited by thermal deposition on the HOPG. The Al_2O_3 growth at RT was studies after the first, third, and fifth cycle. Silver evaporation leads to step decoration with island of 1nm-7nm. On the terraces we find the formation of 2D domain of Ag chains. The features caused by the individual ALD cycles of Al_2O_3 depend on the terrace widths of the HOPG substrate. For small terraces (*100nm) we obtain a growth of 2D domains (20nm-25nm) on the edge steps and in the middle of the terrace. For large terraces (*100nm) we find agglomeration of the precursors on individual nucleation sites. Here 3D islands are formed with a height of up to 5nm in the fifth ALD cycle.

O 89.13 Thu 18:15 H4

HfO_2 grow by ALD on Si(111)-H terminated stepped surface — •Zied Rouissi[1], Massimo Tallarida[2], and Dieter Schmeisser[1] — [1]Applied Physics and Sensors, K.-Wachsmann-Allee 17, D-03046 Cottbus, Germany — [2]ALBA Synchrotron, 08290 Cerdanyola del Vallès, Barcelona, Spain

We studied by STM the growth of HfO_2 on Si (111)-H stepped surface (miscut by 0.5°). The steps are aligned in the [11-2] direction. In order to obtain well defined steps and terraces we prepare the sample by chemical etching in 40% Nh_4F. In our in-situ study we investigate the ALD growth of HfO_2 by TDMAH and H_2O [1-2]. We follow for the first four ALD cycles the distribution of the nucleation sites. We also study the influence of the substrate temperature by comparing the growth within the ALD window at 300K and 580K. We observed that at RT the as-grown HfO_2 forms stripes which are oriented normal to the step orientations. Further growth starts from the step edges and proceeds towards the terraces. Defects created by the etching processes act as nucleation sites for 3D islands. Based on our STM data we are able to correlate the structural changes on that inert and stepped Si(111)-H surface during ALD with experimental [3] and theoretical [4] results obtained for planar Si(100) surfaces.

[1] M. Tallarida et al., Semicond. Sci. Technol. 27, 074010 (2012)
[2] K. Kolanek et al., Thin Solid Films 518, 4688 (2010)
[3] K. Kolanek et al., J. Vac. Sci. Technol. A 31, 01A104 (2013)
[4]L. Riikka et al., J. Appl. Phys.96, 7686 (2004)

O 90: Topological Insulators I

Time: Thursday 14:45–17:15 Location: H10

O 90.1 Thu 14:45 H10

Topological Dirac Semimetal in strained HgTe — •Tomáš Rauch[1], Steven Achilles[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle (Saale), Germany

HgTe, one of the most intensively investigated materials in the context of topological insulators, is a semimetal with zero energy band gap when considered as a three-dimensional material. Applying uniaxial strain in [001] direction changes the situation dramatically [1]. Under compressive strain HgTe becomes a strong topological insulator featuring typical Dirac cone shaped surface states at the $\overline{\Gamma}$ point of the surface Brillouin zone. On the other hand, applying a tensile strain makes HgTe a topological Dirac semimetal with a pair of doubly-degenerate Dirac cones located along the k_z axis of the bulk Brillouin zone.

By combined *ab initio* and tight-binding electronic structure calculations we investigate the bulk and surface electronic properties of three-dimensional HgTe in the topological Dirac semimetal phase. This includes calculating the bulk band structure, topological invariants, and the electronic structure of the (100) surface, at which the associated non-trivial surface states emerge.

[1] T. Rauch *et al.*, Phys. Rev. Lett. **114**, 236805 (2015)

O 90.2 Thu 15:00 H10

Tight-Binding Approach towards an Effective Model for InAs/GaSb Quantum Wells — •Matthias Sitte[1], Karin Everschor-Sitte[1], and Allan MacDonald[2] — [1]Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudingerweg 7, 55128 Mainz — [2]The University of Texas at Austin, Department of Physics, 2515 Speedway, Austin, TX 78712-1192

Topological insulators have attracted a great deal of attention as a new quantum state of matter in the last decade. The first realizations of 2D TIs were HgTe/CdTe quantum well heterostructures, but in recent years another class of semiconductor heterostructures — namely InAs/GaSb quantum wells — was shown to yield 2D TIs as well. Compared to the HgTe/CdTe-based systems they have many advantages, most prominently a continuously tunable band structure via external electric fields and stronger proximity coupling to superconductors. We perform empirical tight-binding calculations on these systems to study how topological properties are changed by varying external control parameters such as electric fields or well thicknesses.

O 90.3 Thu 15:15 H10

Negative Magnetoresistance of TlBi$_x$Sb$_{1-x}$Te$_2$ — •Oliver Breunig, Zhiwei Wang, Fan Yang, Alexey Taskin, and Yoichi Ando — II. Physikalisches Institut, Universität zu Köln

In the family of the ternary II-V-VI$_2$ compounds several materials have been identified as topological insulators. In the n-type TlBiTe$_2$ a topological surface state has been found, yet it is hardly accessible for transport studies due to the overlap with the bulk bands. Theoretical studies suggest that upon substituting Bi by Sb a narrow bulk band gap opens while preserving a single Dirac cone at the Γ point, leading to a possible realization of a bulk-insulating system with an exposed Dirac point.

Single crystals of TlBi$_x$Sb$_{1-x}$Te$_2$ were grown by a modified Bridgman technique using high-purity starting materials. They were characterized by ICP/EDX as well as transport measurements. For intermediate values x we find insulating transport properties and a surprisingly strong negative magnetoresistance. We present our crystal growth results of TlBi$_x$Sb$_{1-x}$Te$_2$ and discuss the origin of the observed large negative magnetoresistance.

O 90.4 Thu 15:30 H10

Landau level spectroscopy of the 3D topological insulator Sb$_2$Te$_3$ — •Stefan Wilfert[1], Oliver Storz[1], Paolo Sessi[1], Thomas Bathon[1], Konstantin Kokh[2], Oleg Evgen'evich Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Sb$_2$Te$_3$ is a prototypical three-dimensional topological insulator (TI) with intrinsic p-doping, which leads to a Dirac point lying well above the Fermi level [1]. We performed energy-dependent quasi-particle interference mapping and scanning tunnel spectroscopy in high magnetic fields up to 12 T on this compound, where both methods allow to obtain the energy dispersion. In contrast to the much more studied TIs Bi$_2$Te$_3$ [2] and Bi$_2$Se$_3$ [3], Sb$_2$Te$_3$ shows Landau levels with both negative and positive Landau level indices. This enables to analyze in more detail the energetic broadening of the Landau levels, which may lead to a better understanding of the physical limits of quantum coherence in this type of materials.

[1] C. Seibel *et al.*, Phys. Rev. Lett. **114**, 066802 (2015).
[2] Y. Okada *et al.*, Phys. Rev. Lett. **109**, 166407 (2012).
[3] T. Hanaguri *et al.*, Phys. Rev. B **82**, 081305 (2015).

30 min. Coffee Break

O 90.5 Thu 16:15 H10

Aharonov-Bohm effect in the 3D topological insulator HgTe — •Johannes Ziegler[1], Dmitriy Kozlov[1,2,3], Dmitry Kvon[2,3], Nikolay Mikhailov[2], Sergey Dvoretsky[2], and Dieter Weiss[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]A.V. Rzhanov Institue of Semiconductor Physics, Novosibirsk, Russia — [3]Novosibirsk State University, Russia

We present our progress in the investigation of the Aharonov-Bohm effect in ring and nanowire structures, fabricated from high-mobility strained 80 nm HgTe films with a wet etching technique. The nanostructures are equipped with topgates to allow tuning of the Fermi level E_f and are measured in a dilution cryostat.

The focus lies on Topological Insulator nanowires, where it is expected that the magnetic flux Φ through the wire leads to both Φ_0 and $\Phi_0/2$ periodic oscillations [1]. Φ_0 $(= h/e)$ periodic oscillations are expected to occur in the ballistic regime for a large range in E_f. For ballistic devices, both minima and maxima of the conductance are expected at $\Phi = \Phi_0/2$ with varying E_f. In the case of diffusive transport, Φ_0 periodic oscillations are expected for E_f close to the Dirac point, while tuning E_f away from the Dirac Point leads to $\Phi_0/2$ $(= h/2e)$ periodic oscillations.

[1] J.H. Bardarson *et al.*, Phys. Rev. L **105**, 156803 (2010)

O 90.6 Thu 16:30 H10

Emergence of quantum spin Hall and half-topological states at Graphene/TMDC heterostructures — •Denis Kochan, Martin Gmitra, Petra Högl, and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, Germany

We discuss orbital and spin-orbital proximity effects emerging in graphene deposited on a monolayer transition-metal dichalcogenides (TMDCs: MoS2, MoSe2, WS2, WSe2) and analyze the impact on spin transport in such graphene/TMDC heterostructures. First-principles investigations show that graphene on MoS2, MoSe2, and WS2 has a topologically trivial band structure, while graphene on WSe2 exhibits inverted bands. The essential low energy physics can be well described by a symmetry inspired realistic tight-binding Hamiltonian. We predict topologically protected helical edge states for graphene zigzag nanoribbons on WSe2, demonstrating the emergence of the quantum spin Hall effect. Our model also features “half- topological states”, which are protected against time-reversal disorder on one edge only. Unlike in pristine graphene, the proximity spin-orbit coupling in graphene on TMDCs is significant (orders of meV), making the predicted effect testable experimentally.

This research was supported by DFG SFB 689, GRK 1570 and by the EU Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

O 90.7 Thu 16:45 H10

Chiral Magnetic Effect in an Interacting Weyl Semimetal — •Matthias Puhr, Semen Valgushev, and Pavel Buividovich — Universität Regensburg, D-93053 Regensburg, Deutschland

We present results of a mean-field study of the chiral magnetic effect in a simple model of a parity-breaking Weyl semimetal. Our model is given by the lattice Wilson-Dirac Hamiltonian with on-site repulsive interaction and a constant chiral chemical potential term. We find a non-trivial behaviour of the chiral magnetic conductivity (CMC) and observe an increase, a decrease and even a change of sign depending on the interaction strength. The absolute value of the CMC never exceeds the value for the non-interacting gapless Hamiltonian. Our model exhibits a phase transition to a phase with spontaneously broken parity (Aoki phase, axionic insulator phase) and we observe a strong suppression of the CMC in the parity broken phase.

O 90.8 Thu 17:00 H10

Negative magneto-resistivity in finite-size samples of Weyl semimetals — Pavel Buividovich, Matthias Puhr, and •Semen Valgushev — University of Regensburg, Regensburg, Germany

We numerically study Chiral Magnetic Effect and magneto-resistivity in a slab of parity-breaking Weyl semimetal modeled by Wilson-Dirac hamiltonian with open boundary conditions and subjected to the external magnetic field parallel to the boundaries. We find that the density of CME current is locally non-zero and strongly localized near the boundaries, where it approaches conventional value $j = \mu_5 B/2\pi^2$. We calculate the magneto-resistivity in a physical setup when parallel magnetic and electric fields are applied to the sample and discuss our results in the context of recent experiments on negative magneto-resistivity in Weyl semimetals.

O 91: Annual General 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 92: Post-Deadline Session

Time: Thursday 19:30–20:30 Location: H1

Contributed Post-Deadline Talks

O 93: Overview Talk: Wilfried Wurth

Time: Friday 9:30–10:15 Location: S054

Invited Talk O 93.1 Fri 9:30 S054

New Science Opportunities with X-Ray Free-Electron Lasers — •Wilfried Wurth — Physik Department und Center for Free-Electron Laser Science, Universität Hamburg — DESY Photon Science, Hamburg

New light sources based on linear accelerators such as the free-electron laser FLASH at DESY in Hamburg in the extreme ultraviolet, the Linac Coherent Light Source LCLS in Stanford and SACLA at SPring-8 in Japan in the x-ray regime, or FERMI at ELETTRA in Trieste as the first fully externally seeded free-electron laser provide ultrashort, extremely powerful short wavelength pulses with unprecedented coherence properties.

With these new sources it is possible to extend the well-established x-ray spectroscopy and scattering techniques for the investigation of the static electronic and geometric structure of matter to probing their evolution after controlled excitation in the time domain.

The talk will give an overview on the physics of these sources and review recent time-resolved x-ray spectroscopy and imaging experiments illustrating the opportunities for the study of ultrafast dynamics at surfaces.

O 94: Ultrafast Surface Dynamics II

Time: Friday 10:30–12:15 Location: S054

Invited Talk O 94.1 Fri 10:30 S054

Time-resolved electron microscopy: probing ultrafast processes at the nanoscale — •Sascha Schäfer — 4th Physical Institute-Solids and Nanostructures, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Ultrafast transmission electron microscopy (UTEM) is a promising technique for the investigation of ultrafast dynamics with nanoscale spatial resolution [1]. In UTEM, a pulsed electron beam with subpicosecond bunch duration is utilized to stroboscopically probe laser-induced processes, using the versatile imaging and diffraction capabilities of electron microscopy. However, up to now, its applicability was limited by the coherence properties of available pulsed electron sources. In the Göttingen UTEM project, we developed nanoscale laser-driven photocathodes, which allow for the generation of highly coherent electron pulses. At the sample position, we achieve electron focal spot sizes down to a few nanometers with a pulse duration of about 300 fs. Such a tightly focused ultrafast probe enables the investigation of fast processes in heterogeneous systems and at interfaces, and I will present some first applications, including the inelastic electron scattering in optical near-fields [2], and the mapping of optically induced structural dynamics at the edge of a single-crystalline graphite membrane.

[1] A. H. Zewail, Science 328, 187-93 (2010). [2] A. Feist, K. E. Echternkamp, J. Schauss, S. V. Yalunin, S. Schäfer, C. Ropers. Nature 521, 200-203 (2015).

O 94.2 Fri 11:00 S054

A remotely driven ultrafast electron source — •Jan Vogelsang[1], Jörg Robin[1], Benedek J. Nagy[2], Péter Dombi[2], Daniel Rosenkranz[1], Manuela Schiek[1], Petra Gross[1], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany — [2]Wigner Research Centre for Physics, 1121 Budapest, Hungary

The combination of high spatial resolution electron microscopes and high temporal resolution laser spectroscopy promises experiments in today unexplored spatio-temporal regimes. However, in such microscopes the time resolution is so far limited to ~100fs: The distance between electron emission site and the sample must be larger than the laser focus radius. This gives rise to electron pulse broadening due to dispersion. Yet, many fundamental photoinduced processes such as coherent charge and energy transport phenomena, e.g. in solar cells, occur on few femtosecond time scales and remain hidden.

Here, we present photoelectron emission from the apex of a gold nanotaper illuminated via grating coupling at a distance of 50μm from the emission site with few-cycle laser pulses (Nano Lett. 15, 4685). Compared to direct apex illumination, we find a fifty-fold increase in electron yield. Point-projection microscopic imaging of Ag-nanowires is performed and spatial localization of the electron emission to a nanometer-sized region is demonstrated. This novel emission scheme allows for arbitrarily small distances between emission site and sample. Hence, it is of immediate interest for miniaturized electron microscopy and diffraction schemes with ultrahigh time resolution.

O 94.3 Fri 11:15 S054

Femtosecond electron dynamics: Accessing the momentum space — •Norman Haag, Johannes Seidel, Lisa Grad, Benjamin Stadtmüller, Mirko Cinchetti, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

Time resolved two-photon photoemission spectroscopy has proven to be a powerful tool to investigate electron dynamics at surfaces on a femtosecond timescale [1]. Combining this method with momentum microscopy [2], a novel tool for angle resolved photoemission, offers the possibility to follow electron dynamics throughout the entire accessible momentum space.

As a prototype system, we have studied the pristine Ag(111) surface as well as a monolayer of Pb grown on Ag(111) with time resolved momentum microscopy. We have chosen these systems as they exhibit either surface states or quantum well states. The significantly different wave function overlap of these states with bulk states of the silver substrate will yield different relaxation dynamics of excited electrons. Analyzing different regions in momentum-space for constant intermediate state energy provides a detailed view of the momentum space dynamics of optically excited electrons.

References

[1] M. Bauer et al., Prog. in Surf. Sc. 90, 319 (2015)
[2] C. Tusche et al., Ultramicroscopy (2015)

O 94.4 Fri 11:30 S054

Novel light source for time- and angle-resolved photoelectron spectroscopy — •Michele Puppin[1], Yunpei Deng[2], Johannes Feldl[1], Chris Nicholson[1], Claude Monney[3], Hendrik Vita[1], Martin Wolf[1], and Ralph Ernstorfer[1] — [1]Fritz-Haber Institut, Berlin, Germany — [2]Paul-Scherrer Institut, Switzerland — [3]University of Zurich, Switzerland

Time- and Angle- Resolved Photoemission Spectroscopy (tr-ARPES) accesses the out-of-equilibrium electronic band structure in the time domain and provides information on coupling and correlation effects between electronic and lattice degrees of freedom as well as on excited state dynamics. These studies benefit from the high counting statistics of light sources with 100s of kHz repetition rate. However, due to their low photon energy (< 6.3 eV), high repetition rate sources were limited so far to investigations at the Brillouin zone center. We have developed an efficient femtosecond source with 500 kHz repetition rate capable of tr-ARPES with XUV pulses, granting access the full Brillouin zone. The key component of this approach is an optical parametric chirped-pulse amplifier (OPCPA) providing intense 30 fs pulses. A simple monochromatization scheme allows selecting a single harmonic at 22.3 eV with 100 meV bandwidth with a photon flux exceeding 10^{11} photons/s. First proof-of-concept tr-ARPES data on transition metal dichalcogenides are presented.

O 94.5 Fri 11:45 S054

Attosecond Delays in the Photoemission from the Layered Crystals Bi_2Te_3 and Non-Centrosymmetric BiTeCl — •Sergej Neb[1], Christian Oberer[1], Walter Enns[1], Norbert Müller[1], J. Hugo Dil[2,3], Evgueni V. Chulkov[4,5], Pedro M. Echenique[4], Walter Pfeiffer[1], and Ulrich Heinzmann[1] — [1]Universität Bielefeld, Germany — [2]Paul-Scherrer-Institut, Villigen, Switzerland — [3]Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne, Switzerland — [4]Donostia International Physics Center (DIPC) and Unidad de Fisica de Materiales CSIC-UPV/EHU, Basque Country, Spain — [5]Tomsk State University, Russian Federation

The availability of single attosecond (as) XUV pulses allows investigating ultrafast electron dynamics on the as time scale by recording slight temporal shifts of the photoelectron streaking in a simultaneously present strong IR field. The physical origin of the observed delays is not yet understood and controversial theoretical models coexist demonstrating our still limited understanding of the fundamentals of the photoemission process. Here we report on as-time-resolved photoemission from the layered crystals Bi_2Te_3 and non-centrosymmetric BiTeCl. The lack of inversion symmetry allows studying relative photoemission delays on differently terminated but well-defined surfaces. Due to reversed layer stacking, photoelectron propagation effects such as the mean free path and the internal effective potential can be determined. However, the measured relative delays cannot be explained by electron propagation alone. Hence effects beyond pure propagation through the layers influence the photoemission dynamics.

O 94.6 Fri 12:00 S054

Pump laser-induced space-charge effects in HHG-driven time- and angle-resolved photoelectron spectroscopy — •Lars-Philip Oloff, Kerstin Hanff, Ankatrin Stange, Gerald Rohde, Florian Diekmann, Michael Bauer, and Kai Rossnagel — Insitut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

The development of fs-pulsed XUV sources such as free-electron lasers or high-harmonic-generation (HHG) sources has opened up a new scientific field for photoelectron spectroscopy in terms of time-resolved pump-probe experiments. While the impact of the high peak brilliance of these novel sources on photoemission spectra has been studied extensively, the effect of high pump fluences has not been investigated systematically yet. In the strong excitation regime, the low photon energy pump pulses may lead to the emission of electrons from the sample via multiple photon absorption, thus directly influencing the electrons ejected by the probe pulse through Coulomb interaction. We have systematically investigated these so called space-charge effects at a HHG source (22.3 eV) for the case of a graphite (HOPG) sample. Specifically, we have studied the influence on the photoelectron energy and momentum distributions as a function of power density, spot size, pump-probe delay, and pump wavelength. The results are interpreted in terms of a simple mean-field model.

O 95: Graphene IV: Electronic Properties and Structure

Time: Friday 10:30–13:00 Location: S051

O 95.1 Fri 10:30 S051

Graphene tunable transparency to tunneling electrons: A direct tool to measure the local coupling. — •Héctor González Herrero[1], Antonio Javier Martínez Galera[2], Miguel Moreno Ugeda[3], Delia Fernández Torre[4], Pablo Pou[4], Rubén Pérez[4], José María Gómez Rodríguez[1], and Iván Brihuega[1] — [1]Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]CIC nanoGUNE, E-20018 Donostia-San Sebastian, Spain — [4]Dept. Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Graphene grown on metals has proven to be an excellent approach to obtain high quality graphene films. However, special care has to be taken in order to understand the interaction of graphene with the substrate since it can strongly modify its properties.

We have grown one monolayer graphene on Cu (111) by using a new technique. By means of low temperature STM/STS experiments, complemented by density functional theory calculations, we have obtained information about the structural and electronic properties of our graphene samples with atomic precision and high energy resolution. Our work shows that depending on the STM tip apex and the tunnel parameters we can get access to either the graphene layer, the copper surface underneath or even both at the same time. Moreover, this approach can also be applied to investigate the interaction of point defects in the graphene layer with the underlying substrate .

O 95.2 Fri 10:45 S051

Excitons and the XNLD of higly oriented pyrolytic graphite and graphene - theory and experiment — •Dominik Legut[1], Robert Laskowski[2], Peter M. Oppeneer[3], Christine Jansing[4], Markus Gilbert[4], Andreas Gaupp[4], Hans-Christoph Mertins[4], Andrey Sokolov[5], Suk-Ho Choi[6], Hud Wahab[7], and Heiko Timmers[7] — [1]IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic — [2]Institute of High Performance Computing, A*STAR, Singapore — [3]Department of Physics and Astronomy, Uppsala, Sweden — [4]FH Münster, Steinfurt, Germany — [5]HZB, Berlin, Germany — [6]Department of Applied Physics, Kyung Hee University, Korea — [7]University of New South Wales Canberra, Canberra BC, Australia

Reflection spectra of the x-ray natural linear dichroism (XNLD) were calculated on highly oriented pyrolytic graphite (HOPG) and graphene. The π- and σ-excitations stemming from the carbon K-edge are considered. It was computed in the single electron picture within the framework of the standart DFT as the first step. For the better descriptions of the core-hole quasiparticle one can model the Slater transition state employing the supercell calculation with partial hole on one of the carbon atoms with the electron charge distributed over the valence states. Another approach is to solve Bethe-Salpeter equations for the many-body electronic effects. The latter approach clearly identify the excitonic features of π- and σ-excitations HOPG. The spectral shape of the reflectance and XNLD of all three modeles are compared with the experimental data.

O 95.3 Fri 11:00 S051

Direct measurement of chiral symmetry breaking in strained graphene by STM — Alexander Georgi[1], •Peter Nemes-Incze[1], Ramon Carillo-Bastos[2], Martin Schneider[3], Dinesh Subramaninam[1], Torge Mashoff[4], Daiara Faria[2,5], Silvia Viola Kusminskiy[3], Dawei Zhai[2], Marcus Liebmann[1], Marco Pratzer[1], Ludger Wirtz[6], Nancy Sandler[2], and Markus Morgenstern[1] — [1]RWTH Aachen Univ. and JARA-FIT, Aachen, Germany — [2]Ohio Univ., Athens, Ohio, USA — [3]Freie Univ. Berlin, Berlin, Germany — [4]Johannes Gutenberg-Univ., Mainz, Germany — [5]Univ. Federal Fluminense, Niterói, Brazil — [6]Univ. of Luxembourg, Luxembourg

The breaking of reflection symmetry has important consequences for pseudospin 1/2 particles, such as those used to describe low-energy excitations in graphene. Here we show that forces exerted by the tip of a scanning tunneling microscope induce mechanical strain on sub-nm length scales that acts as a gauge field breaking the chiral symmetry of the system. The parity violation manifests itself as a redistribution of the local density of states between the two sublattices by up to 30%. The effect can be understood as a pseudospin polarization due to a pseudo-Zeeman shift produced by the strain induced pseudo-magnetic field. This interpretation is supported by tight binding simulations and effective Dirac model calculations. The tunable pseudo-magnetic field might be used for the ultra fast separation of electrons of different valleys providing a switchable valley filter as a basic element for valleytronics.

O 95.4 Fri 11:15 S051

Layer symmetry breaking field and conductivity in graphene twist bilayer — •Nicolas Ray, Sam Shallcross, and Oleg Pankratov — Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

The rich electronic structure of the graphene twist bilayer includes both a decoupled large angle limit and a strongly coupled small angle limit [1]. We consider the in-plane conductivity via a linearised Boltzmann equation [2] over the full angle range, both with and without a layer-perpendicular electric field. The layer perpendicular electric field is shown to lead to a strong suppression of conductivity at certain "hot spots" in the twist angle and energy phase space.

[1] S. Shallcross et al., Phys. Rev. B 87, 245403, 2013; [2] E. Mariani et al., Phys. Rev. B 86, 165448, 2012.

O 95.5 Fri 11:30 S051

How partial dislocations may make bilayer graphene both an insulator and a conductor — Heiko Weber[1] and •Sam Shallcross[2] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7 A3, 91058 Erlangen, Germany — [2]Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

Recently imaged partial dislocations in bilayer graphene [1] have been shown to have a profound impact on transport properties for the case of bilayer graphene on SiC [2]. We demonstrate that the presence of only a few partial dislocations in high quality suspended bilayer graphene can both destroy the intrinsic minimal conductivity of the structurally perfect bilayer, or even enhance it, depending only on the configuration of the partials. The provides a natural explanation for the peculiar behaviour of suspended bilayer graphene, in which seemingly very similar samples are found to be either insulating or conducting in nature.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature 505, 533 (2014). [2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Physics 11, 650 (2015).

O 95.6 Fri 11:45 S051

Electronic structure of partial dislocations in bilayer graphene — Dominik Weckbecker and •Sam Shallcross — Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

We present electronic structure calculations for the partial dislocations recently imaged in bilayer graphene on SiC [1,2]. We use an effective field method which allows us to treat both a realistic experimental situation of many disordered dislocations in a sample area of a square micrometer as well as model systems in which the dislocations are ordered. We find near the Dirac point a charge pooling on the bilayer graphene segments, as well as a curious energy dependent localization on the partial lines and partial nodes. We consider the presence of an external out-of-plane magnetic field and identify current circulations associated with partial lines.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature 505, 533 (2014). [2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Physics 11, 650 (2015).

O 95.7 Fri 12:00 S051

Deformation in graphene and few layer graphenes: interlayer gauge fields and optical deformations — •Nicolas Ray[1], Fabian Rost[1], Reena Gupta[2], Sangeeta Sharma[2], Oleg Pankratov[1], and Sam Shallcross[1] — [1]Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany — [2]Max-Planck-Institute for Microstructure Physics, Weinberg 2, 06120 Halle, Germany

We present a general theory of deformations in graphene and few layer graphenes. In single layer graphene we consider both acoustic and optical deformations, and show that the latter can generate chiral gap opening fields. For the case of few layer graphenes we derive a general interlayer gauge term that relates the local stacking vector to an off-diagonal non-Abelian field. We show that this general result reduces to well known cases such as the Bernal or twist graphene bilayer, but can also be used to treat more complex situations such as partial dislocations in bilayer graphene.

O 95.8 Fri 12:15 S051

Substrate nanofacets as a stamp for graphene charge carrier modulations — •Jan Honolka[1], Martin Vondracek[1], Ladislav Fekete[1], Jaromir Kopecek[1], Jan Lancok[1], Dipankar Kalita[2], Johann Coraux[2], and Vincent Bouchiat[2] — [1]Institute of Physics, ASCR, CZ-Prague — [2]Department Nanosciences, CNRS, F-Grenoble

We report on 1D quasiperiodic modulations of graphene electron doping, probed by spatial mapping of the electronic band structure in wave-vector-resolved photoemission microscopy (k-PEEM).

Sampling local topography and diffraction, we show that a nanometer-scale periodic structuration and electronic doping by several 0.1eV can be achieved straightforwardly in graphene, as-grown by CVD on high-index vicinal copper. The pattern consists of a rooftop-like alternance of Cu facets of distinctive symmetries, formed by surface energy minimization at the atomic scale, which drives copper and carbon mass-transfers during high-temperature CVD.

The general concept of this work can be extended towards other chemical vapor deposited 2D systems of current interest such as semiconducting transition metal dichalcogenides, e.g. MoS_2, insulating hexagonal boron nitride (h-BN) monolayers, and respective hybrid structures.

O 95.9 Fri 12:30 S051

Fermi surface nesting in the graphene twist bilayer — •Maximilian Fleischmann, Dominik Weckbecker, Nicolas Ray, Oleg Pankratov, and Sam Shallcross — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

Two mutually rotated layers of graphene exhibit an electronic structure that depends profoundly on the rotation angle of the two layers [1]. This rich electronic structure invites the possibility of significant band engineering control in the small angle limit [2]. We demonstrate that the small angle limit exhibits a massive Fermi surface nesting in the presence of a perpendicular electric field of strength greater than ~ 100 mV/Å. We describe in detail the unusual band topology in this nested region of the energy field phase space, and discuss some of the many body effects likely to be induced by such strong Fermi surface nesting.

[1] S. Shallcross et al., Phys. Rev. B **87**, 245403, 2013.

[2] D. Weckbecker et al., *submitted*

O 95.10 Fri 12:45 S051

Force-induced dynamic STM mapping and picking of free-standing graphene membranes — •Bernd Uder, Wolf-Rüdiger Hannes, and Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany

Scanning Tunneling Microscopy (STM) of freely suspended membranes only a few atomic layers thick is inherently challenging. Membrane and tip instabilities are easily induced and must be controlled by careful adjustment of scan and regulation parameters. So far only little STM work has been reported on this surface type. We demonstrate seamless imaging of few-layered suspended graphene, from $10\mu m$ x $10\mu m$ scan width down to 25nm x 25nm. On the scale of 5 - 10nm, we observe corrugations rippled in one dimension. Larger structures are resolved by choosing scan parameters such that vibrational modes are triggered in certain reproducible regions, possibly corresponding to monolayer regions or fragments. Bias voltage ramps are employed for controlled and reversible membrane picking with the observation of flipping processes of the rippled structure.

O 96: Structure of Solid/Liquid Interfaces II

Time: Friday 10:30–13:00 Location: S052

O 96.1 Fri 10:30 S052

Adsorption and desorption of water on protein-repelling self-assembled monolayers — •Mustafa Sayin[1], Alexei Nefedov[2], and Michael Zharnikov[1] — [1]Institute of Applied Physical Chemistry, University of Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — [2]Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

We studied kinetics and thermodynamics of water adsorption and desorption as well as wetting and nucleation behaviors of water on a series of model organic surfaces, formed by oligo(ethylene glycol) substituted alkanethiolate (OEG-AT) self-assembled monolayers. The ultimate goal of the study was to get a better understanding of the mechanism behind the inertness of poly(ethylene glycol) and OEG based organic surfaces with respect to biofouling and protein adsorption. Varying the water coverage and the capability of surface hydration, by suitable design of the of the OEG-ATs molecules and respective self assembled monolayers, we monitored transfer from the hydration to wetting regime, distinguishing between the hydration and interfacial phases and deriving specifically their parameters. The bonding character of the hydration phase as well as the structure and morphology of the interfacial phase were investigated by high resolution X-ray photoelectron spectroscopy, in situ infrared reflection absorption spectroscopy, and near edge X-ray absorption fine structure spectroscopy. The kinetics of the water desorption was studied by thermodesorption spectroscopy.

O 96.2 Fri 10:45 S052

A High-Dimensional Neural Network Potential for Water at Zinc Oxide: First Applications to Non-Polar Interfaces — •Vanessa Quaranta, Matti Hellström, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Germany

Zinc oxide (ZnO) is an important material in surface science, which has many applications in different fields [1]. In most of these applications, water is ubiquitous playing a crucial role. To understand these processes at the atomic level, realistic structural models of water/ZnO interfaces are crucial. However, the required large systems often containing thousands of atoms dramatically limit the application of *ab initio* techniques. In recent years, artificial neural networks (NNs) have emerged as a powerful efficient method to provide accurate PESs for a variety of systems [2]. Here, we report first results for a DFT-based NN potential constructed for liquid water/ZnO interfaces. In particular, the structural and dynamical properties of interfacial water molecules interacting with non-polar ZnO surfaces will be presented.

[1] Ch. Wöll, *Progr. Surf. Sci.* **82**, 55 (2007).
[2] J. Behler, *Phys. Chem. Chem. Phys.* **13**, 17930 (2011).

O 96.3 Fri 11:00 S052

Ab-initio molecular dynamics simulations on wet alumina-/isopropanol solid/liquid interfaces — •Paul Schwarz und Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

The solid/liquid interface of wet and hydroxylated α-alumina/isopropanol is studied using ab-initio Car-Parrinello molecular dynamics (CPMD) simulations. For the alumina slab three different surface models are taken into account: a termination with a full hydroxyl layer (**hyd**), an aluminum termination with dissociated water molecules to saturate undercoordinated surface sites (**w1**) and a third termination with adsorbed water molecules between the OH groups of the **w1** structure (**w2**).

Simulations of the **w2** slab show that the additional water molecules induce recombinations events on the surface, leading to the protonation of several OH groups and thereby to the formation of water molecules on top of the aluminum atoms. The occurrence and distribution of these newly formed water molecules is analyzed, as well as proton hopping events on the surface. We show that the proton hopping is energetically driven and correlates with an increased number of H-bonds. Recombination events are also found for the **w1** slab after adding isopropanol, whereas the **hyd** surface remains unchanges. Finally, the influence of the surface termination on the structure of the isopropanol liquid will be discussed.

O 96.4 Fri 11:15 S052

A joint *first principles* and ATR-IR study of the vibrational properties of interfacial water at semiconductor-water solid-liquid interfaces — •Lei Yang[1], Stefanie Tecklenburg[1], Fang Niu[1], Andreas Erbe[1], Stefan Wippermann[1], Francois Gygi[2], and Giulia Galli[3] — [1]Max-Planck-Institut für Eisenforschung — [2]University of California, Davis — [3]University of Chicago

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. We carried out joint ATR-IR spectroscopy measurements and *ab initio* molecular dynamics simulations of the vibrational properties of interfaces between liquid water and prototypical semiconductor substrates. In particular, the Ge(100)/H_2O interface is shown to feature a reversible bias potential dependent surface phase transition. Our study highlights the key role of coupled theory-experimental investigations on well controlled and characterized interfaces, in order to develop robust strategies to interpret experiments and validate theory. The authors wish to thank T. A. Pham for helpful discussions. G. G. and F. G. acknowledge DOE-BES Grant No. DE-SS0008939.

O 96.5 Fri 11:30 S052

A first-principles study on the phase stability of ZnO(0001)-Zn surfaces — •Suhyun Yoo, Mira Todorova, and Joerg Neugebauer — Department of Computational Materials Design, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany

Zinc oxide is a wide bandgap semiconductor, which is intensively studied due to its applications in different fields, such as (photo-)catalysis, protective coating, optoelectronics and others. Knowledge of the surface structures which form when ZnO surfaces come into contact with different environments (gas phase, liquid) and are thermodynamically stable is important in the context of most of these applications. Focusing on the polar Zn terminated ZnO(0001) surface we combine density functional theory (DFT) calculations with thermodynamic concepts to study how the stability of surface phases forming on ZnO(0001)-Zn surfaces [1] is influenced by (i) the improved description of the band gap, as achieved by DFT-HSE calculations and (ii) the contact with an aqueous environment. Modelling liquid water by an implicit solvation model [2], we utilize our recent electrochemical approach [3] to construct a surface Pourbaix diagrams for this surface.

[1] M. Valtiner, M. Todorova, G. Grundmeier, and J. Neugebauer, Phys. Rev. Lett. 103, 065502 (2009).

[2] K. Mathew, R. Sundararaman, K. Letchworth-Weaver, T.A. Arias, and R.G. Hennig, J. Chem. Phys. 140, 084106 (2014).

[3] M. Todorova and J. Neugebauer, Phys. Rev. Applied 1, 014001 (2014).

O 96.6 Fri 11:45 S052

Water adsorption on clean bimetallic Pt-Ru(0001) surfaces - a low-temperature UHV-STM investigation — •Martin Schilling, Sylvain Brimaud, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm

A detailed understanding of the elementary electrochemical/-catalytic processes on catalytically relevant electrode surfaces requires the characterization of the solid | liquid interface, including the water-metal interaction and the influence of coadsorbed species. The water-metal interaction has been studied in detail earlier, using model systems consisting of ice layers adsorbed on monometallic single crystal surfaces [1].

Here, we present results of a scanning tunnelling microscopy (STM) study on the structure of H_2O on 2D bimetallic PtRu model electrodes. H_2O was deposited under well-defined conditions in ultrahigh vacuum (UHV) at low sample temperatures (100 - 130 K) on Pt modified Ru(0001) single crystal surfaces. In addition to adsorption on the clean metal surfaces, also structural effects of pre- or coadsorbed species on the overlayer structure were investigated. The structures were characterized by STM in the temperature range of 100 K to RT. Depending on the Pt-Ru surface structure, the conditions of H_2O dosing and the presence of coadsorbates we identified different trends for the resulting molecular arrangements of the adsorbate. The influence of substrate-molecule and molecule-molecule interactions is discussed based on the Pt modified Ru(0001) substrate.

[1] J. Carrasco *et al.*, *Nat. Mater.* **11** (2012) 667

O 96.7 Fri 12:00 S052

Water adsorption on Pt(111): water-water vs. water-metal interaction — •Maryam Naderian and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89081 Ulm/Germany

Adsorbed water layers typically form hydrogen-bonded networks at surfaces at low temperatures. The stability of these water layers at solid surfaces is thus governed by a delicate interplay between water-substrate and water-water interactions [1]. Using density functional theory (DFT) calculations, we address the importance of water-water vs. water-metal interactions in the adsorption of water on Pt(111). To get a reliable description of the water-metal system, it is crucial to include dispersion effects in the DFT calculations [2].

The initial steps of the formation of hydrogen-bonded networks have been studied using ab initio molecular dynamics simulations of water adsorption on water-precovered Pt(111). The water-metal interaction has been modified by using Pt-terminated bimetallic surfaces. Ligand and strain effects lead to a variation of the reactivity of the Pt atoms which also influences the balance between water-water and water-metal interaction. The consequence of this variation on the resulting water structures will be discussed in detail.

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

[2] K. Tonigold and A. Groß, J. Comput. Chem. **33**, 695 (2012).

O 96.8 Fri 12:15 S052

Mapping the stabilities of two-dimensional water polymorphs using dispersion-corrected DFT — •Tanglaw Roman and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

The properties of the contact layer of water or ice on solid surfaces are still not fully understood. The questions that require answers include: How ice-like is water close to a solid surface? How realistic are hexagonal bilayer-based models in describing interfaces with water, both on hexagonal close-packed surfaces and on surfaces of other symmetries? How dense is water at these interfaces? What is the most stable form of ordered water in two dimensions? How different is 2D from 3D crystalline water, and how does the transition go? Which physical factors may contribute to the formation of a water lattice with another symmetry? In response to these, we present a systematic sweep of structural possibilities of water in two dimensions using density functional theory with dispersion corrections, screening one and two-layer structures over different symmetries. Starting with free-standing models, calculations yield structures that differ from those previously reported using classical molecular dynamics, and include several structures which we find more stable than the traditional hexagonal bilayer. Results are discussed with respect to observed water structures confined within graphene sheets, and on how these impact our understanding of water structures at solid surfaces of varying symmetries and interaction strengths.

O 96.9 Fri 12:30 S052

Water adsorption at different noble metal/solution interfaces — •Yujin Tong, Martin Wolf, and R. Kramer Campen — Fritz-Haber-Institut, Abt. Physikalische Chemie, 14195 Berlin, Germany

In aqueous electrochemistry water molecules at the electrode/solution interface determine the structure of the electric double layer, mediate charge transfer mechanisms, and are the reactive species in water electrolysis. Hence gaining a molecular level picture of water structure at the electrode/solution interface, and following its change as a function of electrode potential, is of both fundamental and practical importance. However, achieving such insight via most experimental techniques is challenging. Vibrational sum frequency spectroscopy, owning to its unique selection rules, can selectively probe the structure of water molecules at the electrode/solution interface. Using VSF spectroscopy we here show that: 1). On gold electrodes over a wide range of potentials there are hydrophobic water molecules oriented in such a way that one of their OH groups point towards the gold. 2). After partial oxidation of the gold surface, apparent via cyclic voltammetry and ex-situ characterization via VSF spectroscopy of low frequency Au-O modes, the gold surface becomes hydrophilic and this population of water disappears.

O 96.10 Fri 12:45 S052

Understanding the Structure of Liquid Water at Copper Surfaces — •Suresh Kondati Natarajan and Joerg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Germany

Solid-liquid interfaces are of fundamental importance in many fields like electrochemistry, corrosion science and heterogeneous catalysis. While in experiment it is often very challenging to obtain detailed information at the atomic level, a wealth of knowledge is in principle available from molecular dynamics (MD). Ab initio MD simulations provide the most reliable description of these systems, but they are severely limited due to the high computational costs associated with studying large "realistic" interfaces. In this talk, a neural network (NN)-based potential for the copper-water interface fitted to density functional theory (DFT) data will be presented which enables to overcome this limitation. Employing this NN potential, we demonstrate that sufficiently long simulations can be carried out allowing to analyze the structural and dynamical properties in detail.

O 97: Nanostructured Surfaces and Thin Films

Time: Friday 10:30–12:30 Location: S053

O 97.1 Fri 10:30 S053

High-quality Ru(0001) thin films by magnetron sputter deposition for ceria inverse model catalysts — •Meikel Wellbrock, Marc Sauerbrey, Jan Höcker, Marco Schowalter, Jon-Olaf Krisponeit, Jens Falta, and Jan Ingo Flege — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee, 28359 Bremen

The investigation of model systems in heterogeneous catalysis with surface science methods typically requires the use of single crystal substrates. Offering enhanced experimental flexibility at lower costs, thin films prepared by magnetron sputter deposition, an industrially scalable process, represent an attractive alternative. In this study, high-quality, 80 nm thin Ru(0001) films were sputter-deposited on *c*-plane sapphire and then employed as substrates for the subsequent growth of cerium oxide for surface catalysis. After thermal treatment, atomic force microscopy (AFM) and low-energy electron microscopy (LEEM) showed the Ru thin films to be atomically flat over several micrometers, superior to commercially available Ru single crystals. Sequentially, ceria was grown by evaporation of metallic Ce in an oxygen ambient at elevated temperature and monitored *in situ* by LEEM. Contrary to the studies involving single crystal substrates, large, triangular, and smooth CeO_2(111) islands were observed to nucleate exclusively at randomly distributed v-shaped surface defects (v-pits), determining their azimuthal orientation. Together with the narrow height distribution as revealed by *ex situ* AFM, these microparticles represent a well-suited model system for the study of surface chemical reactions over ceria inverse model catalysts.

O 97.2 Fri 10:45 S053

Investigation of monolayer-thick ZrO_2 films created by sputter deposition — •Peter Lackner, Joong-Il J. Choi, Ulrike Diebold, and Michael Schmid — Institute of Applied Physics, TU Wien, Vienna, Austria

Investigating zirconia (ZrO_2) is challenging due to its high band gap. As an insulator it is not accessible to measurement methods relying on electronic conduction, such as scanning tunneling microscopy (STM), at room temperature. To circumvent this issue, ultrathin ZrO_2 films can be studied [1]. However, the very low vapor pressure of zirconium makes deposition slow when using evaporation in ultrahigh vacuum (UHV). We therefore present an UHV-compatible sputter source similar to [2], which can be used to deposit ZrO_2 thin films of any desired thickness.

By variation of film thickness and annealing temperature a continuous and well-ordered film can be produced. We present STM, LEED and XPS results on ZrO_2 films with a thickness of one to 7.5 monolayers. On Rh(111), different surface reconstructions are observed for every layer up to five monolayers. Films with a thickness of five or more monolayers show stripes on the surface, which are indicative of bulk-terminated monoclinic or tetragonal ZrO_2.

[1] Meinel *et al.*, Phys. Rev. B 74, 235444 (2006).

[2] Mayr *et al.*, Rev. Sci. Instrum. 84, 094103 (2013).

O 97.3 Fri 11:00 S053

Microstructure of Yttrium Oxide Deposited by Reactive RF Magnetron Sputtering with Different Oxygen Inlet Flux — •Yiran Mao, Jan Engels, Anne Houben, Jan Coenen, Marcin Rasinski, Jonathan Steffens, and Christian Linsmeier — Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany

Yttria (Y2O3) is a well-known ceramic material extensively used in industry and material science applications. Reactive magnetron sputtering is one of the methods to produce Y2O3 coatings. The influence of the oxygen inlet flux on the Y2O3 film microstructure grown by reactive radio-frequency magnetron sputtering was investigated. The oxygen inlet flux showed a hysteresis behavior effect on the deposition rate. With a low oxygen flux, the so called metallic mode process with a high deposition rate (up to 1.4 *m/h) was achieved, while with a high oxygen flux, the process was considered to be in the reactive mode with low deposition rate (˜20 nm/h). The metallic mode layers represented a mixture of different crystal structures including the metastable monoclinic phase and the stable cubic phase, while the reactive mode products showed a pure monoclinic phase structure. Comparing the reactive mode layers, the metallic mode layers showed dense structures with less porosity. Annealing at 600 °C for 15 h caused a phase transformation from monoclinic phase to cubic phase for both reactive mode and metallic mode. For metallic mode layers, cracks are formed due to the thermal expansion coefficient difference between Y2O3 and the substrate which was not seen in reactive mode.

O 97.4 Fri 11:15 S053

Comparative study of amorphous hydrogenated carbon (a-C:H) layers on Si (100) and high-density polyethylene (HDPE) — •Christian B. Fischer, Alberto Catena, and Stefan Wehner — Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany

Silicon and high-density polyethylene (HDPE) have been gradually covered by thin a-C:H films with acetylene-plasma to study the interlayer forming behavior between the base material and carbon coating. Two different carbon coatings, one with indirect (f-type) and one with direct (r-type) deposition, were realized. Surface characteristic studies by atomic force microscopy (AFM) showed an unexpected similar morphology for both types and materials. The analysis of average height and area for single evolving grains over uniformly textured protrusions at the bottom revealed a smaller amount of carbon deposition for the f-type than for the r-type to obtain similar morphologies independently of the chosen basic material. The average grain area increases for all f- and r-depositions. The average grain height increases in the beginning and approaches a level with nearly constant height. Furthermore, the values of the average grain heights are correlated to the values of the average grain areas and are localized in a limited area, indicating a given regularity throughout the different carbon depositions.

O 97.5 Fri 11:30 S053

Remote plasma treatment as a method to improve the surface conductivity of bipolar plates for fuel cells — •Tatiana Fedosenko-Becker[1,2], Nicolas Wöhrl[1], Volker Buck[1], and Mario Gillmann[3] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]University of Wuppertal, Wuppertal, Germany — [3]ZBT GmbH - The fuel cell research center, Duisburg, Germany

Fuel cells are promising alternative energy sources, therefore they have recently earned scientific interest. However they are not without deficiencies, since during fabrication of carbon/polypropylene (PP) composite bipolar plates (BP) the PP is enriched at the surface reducing the electrical conductivity and the efficiency of the fuel cells. The surface conductivity can be improved by selectively etching the PP from the surface by plasma treatment, using the plasma source CYRANNUS by iplas in remote mode. A detailed investigation of the properties of BP, of plasma processes during the treatment and the influence of the process parameters was done.

It was shown that plasma treatment of BP is a suitable method to decrease the surface resistance without causing mechanical damage to the surface. The most suitable experimental parameters for this task were found. Using FTIR and Raman spectroscopy it was shown that PP and nanocrystalline graphite is removed from the surface. The experimental parameters, such as plasma chemistry, pressure, treatment time, distance from plasma, which provide the best conductivity of the BP, were found.

O 97.6 Fri 11:45 S053

Study of Solid Electrolyte Interphase layer in Sodium-Ion Batteries — •Liang-Yin Kuo[1], Payam Kaghazchi[1], and Bing-Joe Hwang[2] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Department of Chemical Engineering, National Taiwan University of Science and Technology, No.43, Sec. 4, Keelung Rd., Taipei 106, Taiwan

Sodium (Na)-ion batteries are considered as alternative to Li-ion batteries. Sodium is abundance in the earth*s crust and the distribution of sodium mineral salts is widespread. In this work, we present a combined in situ surfaced-enhanced Raman spectroscopy (in situ SERS) and density functional theory (DFT) study on the solid electrolyte interphase (SEI) layer over the surface of Sn anodes in Na-ion batteries. Our in situ SERS measurements show that the main components of the SEI layer during Na-ion insertion/extraction are Na2O (peaks around 479 cm-1 and 597 cm-1) and Na2CO3 (peak around 1080 cm-1). Afterwards, we will discuss our DFT results on electronic and atomic structure as well as the mechanism of Na diffusion through Na2O and Na2CO3.

O 97.7 Fri 12:00 S053

Chemical vapor deposition and infiltration for the production of tungsten fiber reinforced tungsten composite material — •Martin Aumann[1], Jan Willem Coenen[1], Hanns Gietel[2], Till Hoeschen[2], Johann Riesch[2], Klaus Schmid[2], Rudolf Neu[2], and Christian Linsmeier[1] — [1]Forschungszentrum Juelich GmbH, Institut für Energie- und Klimaforschung, 52425 Juelich — [2]Max-Planck-Institut für Plasmaphysik, 85748 Garching

Due to its high melting point, high corrosion resistance and its preferable properties in terms of hydrogen retention, tungsten is a promising candidate in future nuclear fusion devices. However, the mechanical behavior of tungsten is crucial, as it is inherently brittle at room temperature. As possibility to overcome this brittleness, a composite material can be formed, which shows pseudo-ductility and therefore avoids catastrophic failure of the material. A possibility to produce such a Wf/W-composite is chemical vapor deposition and chemical vapor infiltration, where tungsten is deposited on thin tungsten wires through the reaction of WF6 and H2. With ongoing infiltration time, pores are formed between the fibers, which decrease in size through the chemical reaction. For better process understanding, a pore model was established, which solves the mass balance inside the pore and the resulting pore diameter simultaneously. It shows a significant difference in diameter for longer infiltration times. This behavior shall be investigated in experiments with an experimental pore, which is similar to the simulated one. Furthermore also kinetic investigations on the chemical surface reaction are carried out to increase the process understanding.

O 97.8 Fri 12:15 S053

Simulation of oblique angle deposition — •Christoph Grüner, Jens Bauer, Stefan Mayr, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig, Germany

Computer simulations are a powerful tool to study thin film growth phenomena. Here, application of simulations focuses on understanding and controlling atomistic processes during glancing angle deposition in order to create nanostructures with unique new physical properties and functionalities. Ballistic deposition models are used to describe kinetics and morphology of film growth [1]. Such simulation outcomes depend strongly on the implementation of the sticking process and the choice of the simulation grid geometry [2]. Focusing on glancing angle deposition, different issues of simple grid based simulations are studied. Shape and tilt angle of the deposited nanostructures are investigated as well as the porosities of the complete films. The benefit of using cluster particles is discussed.

[1] A.-L. Barabasi and H.E. Stanley, Fractal Concepts in Surface Growth, Cambridge Univ. Press, Cambridge 1995

[2] B. Tanto, C. F. Doiron, and T.-M. Lu, Phys. Rev. E 83 (2011), 016703

O 98: Organic-Inorganic Systems V: Adsorption on Metals

Time: Friday 10:30–13:15 Location: H24

O 98.1 Fri 10:30 H24

Thiolate versus Selenolate: Structure, Stability, and Charge Transfer Properties — •Tobias Wächter[1], Jakub Ossowski[2], Laura Silies[3], Martin Kind[3], Agnieszka Noworolska[2], Florian Blobner[4], Dominika Gnatek[2], Jakub Rysz[2], Michael Bolte[3], Peter Feulner[4], Andreas Terfort[3], Piotr Cyganik[2], and Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — [2]Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Krakow, Poland — [3]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, Max-von-Laue-Straße 7, 60438 Frankfurt, Germany — [4]Physikdepartment E20, Technische Universität München, 85747 Garching, Germany

Self-assembled monolayers (SAMs) of 6-cyanonapthalene-2-thiolate and -selenolate were prepared on Au(111) and characterized by several complementary spectroscopic techniques. The exact structural arrangements in both types of SAMs are somewhat different, but at the same time they have similar packing densities and molecular orientations. This permitted reliable competitive exchange and ion-beam-induced desorption experiments which provided unequivocal evidence for a stronger bonding of selenolates to the substrate as compared to the thiolates. Regardless of this difference, the dynamic charge transfer properties of both adsorbates were found to be nearly identical, as determined by the core-hole-clock approach, which is explained by a redistribution of electron density along the molecular framework, compensating the difference in the bond strength.

O 98.2 Fri 10:45 H24

In-situ LEEM investigation of the growth of organic monolayers on metal surfaces — •Janina Felter, Caroline Henneke, Jana Wolters, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology, Germany

The adsorption of organic molecules on metal surfaces are of highest relevance for applications in the field of organic electronics and for fundamental studies of the interaction mechanisms. In particular, a deep understanding of the nucleation and the formation of the first molecular layer is necessary since this layer acts as a template for further growth and determines the electronic properties of the interface. By using LEEM, PEEM and μLEED, we studied the growth dynamics of Copper-II-phthalocyanine (CuPc) and 1,4,5,8-naphthalene-tetracarboxylic-acid dianhydride (NTCDA) monolayers on low-indexed metal surfaces in-situ and in real-time. Besides others, we have observed the transformation of CuPc domains into each other during and after deposition on Ag(111). In an ongoing PEEM-based ARPES study, we also investigate the electronic properties of these metal-organic interfaces.

O 98.3 Fri 11:00 H24

Multiple molecular templates induced by dehydrogenation of a benzoquinone derivative on Cu(111) — •Giuseppe Mercurio[1], Nils Wind[1], Simon Weiss[2,3], Serguei Soubatch[2,3], Frank Stefan Tautz[2,3], and Wilfried Wurth[1,4] — [1]Physics Department and Center for Free-Electron Laser Science, University of Hamburg, Hamburg, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany — [3]JARA - Fundamentals of Future Information Technology, Germany — [4]DESY Photon Science, Hamburg, Germany

Organic layers on metal surfaces self-organize in a great variety of different surface templates depending on the intermolecular and molecule-metal interactions. The design of a molecular building block with specific structural and chemical properties needs to account for possible chemical modifications (e.g. dehydrogenation) upon deposition on a reactive substrate. In this context a fundamental understanding of the molecule/metal interface before and after dehydrogenation of the selected molecular unit is essential. To this end DHBQ (2,5-dihydroxyl-benzoquinone), a prototypical molecular building block for metal-organic networks, was investigated on the Cu(111) surface. It was found that the dehydrogentation of DHBQ can be thermally activated. Moreover, depending on the degree of dehydrogenation of the molecular layer different superstructures form on the surface. These different molecular phases were investigated by means of x-ray photoemission spectroscopy, low-energy electron diffraction and normal incidence x-ray standing wave.

O 98.4 Fri 11:15 H24

Structure formation of tetramantane[121] on copper(111) — •Marvin Stiefermann[1], Daniel Ebeling[1], Peter Schreiner[2], and André Schrimeisen[1] — [1]Institut für Angewandte Physik der Justus-Liebig-Universität Gießen — [2]Institut für Organische Chemie der Justus-Liebig-Universität Gießen

Nanodiamonds are nanometer sized hydrocarbon molecules, which exhibit a diamondlike structure. As for other nanosized carbon materials (e.g. nanotubes or nanoribbons) diamondoids are discussed to exhibit tunable electronic properties[1]. For future applications in nanoelectronics it is therefore inevitable to study the interaction between diamondoids and solid substrates. Here, we studied the structure formation of tetramantane[121] on a close packed metal substrate with low temperature scanning tunneling microscopy. Tetramantane was evaporated at room temperature under UHV conditions onto a clean copper(111) surface using a self-constructed molecule gun. We observed that tetramantane forms islands on copper(111). Furthermore, we discovered different phases within these islands, which show commensurability with the substrate.

[1] Adhikari et al, Nanotechnology, Volume 26, Number 3, 035701,(2015)

O 98.5 Fri 11:30 H24

On the Temperature-dependent Behavior of Ultrathin Ethylene Carbonate Films on Graphite(0001) — •Maral Bozorgchenani[1], Florian Buchner[2], and R. Jürgen Behm[1,2] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — [2]Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, D-89081 Ulm, Germany

The interaction of ethylene carbonate (EC) with graphite(0001) as a model for the anode|electrolyte interface in Li-ion batteries was investigated under ultrahigh vacuum conditions. X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectroscopy (FTIRS) were employed. After vapor deposition of a monolayer on graphite at 80 K the XP C1s and O1s spectra reveal the adsorption of intact adsorbed molecular adsorbates. Upon slow annealing the intensity of the XP signals related to EC drastically decreases in the temperature range between 190 and 210 K, mainly due to desorption. Subsequently, peaks with low intensity are still visible, which is related to decomposition products on the surface. FTIRS measurements at 80 K demonstrate modes of molecularly adsorbed EC. Difference spectra (background of the EC covered surface) recorded upon annealing reveal the evolution of bands with positive amplitudes (120 - 210 K) which are related either to molecular rearrangement effects or the formation of new species, and with negative amplitudes due to the loss of EC. At 210 K no EC is detected any more. The nature of the EC decomposition products is discussed and a comparison with our previous results on Cu(111) is given.

O 98.6 Fri 11:45 H24

Carbene based molecular anchors on metal surfaces — •Bibek Adhikari[1], Sheng Meng[2], and Maria Fyta[1] — [1]Institute for Computational Physics, Stuttgart, Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing, China

N-hetero-cyclic carbenes (NHCs) are emerging as an alternative class of molecules to thiol-based self-assembled monolayers (SAMs). A carbon-gold bond is stronger than the sulfur-gold bond, making the carbene-based self-assembled monolayers much more stable in harsh environmental conditions. In this work, we have functionalized tiny hydrogenated diamond-like cages, known as diamondoids, using NHCs in order to prepare highly stable self assembled monolayers (SAMs) of diamondoids on metal substrates. Using quantum-mechanical simulations, we were able to extract the structural and electronic properties of the carbene-mediated diamondoid SAMs on metal surfaces. Two different configurations for the carbene-functionalized diamondoids are considered and attached on gold, silver, and platinum surfaces. The binding energy of S-Ag, S-Au, S-Pt and the comparison on the differences between thiol-metal and carbene-metal bonds are reported. A preferential binding to platinum surfaces was found, while a modulation of the work function in all cases was clear. We mainly focus on the binding characteristics and stability of the NHC-mediated diamondoid SAMs. The surface morphology of all NHC-based diamondoid SAMs was shown through the simulated STM images which show characteristic features of each surface.

O 98.7 Fri 12:00 H24

Beyond the hexagon: Non-alternant aromatic molecules on metal surfaces — Benedikt P. Klein, Philipp Müller, Johanna Schepp, Falk Niefind, Malte Zugermeier, Maik Schöniger, Martin Schmid, and •J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

The interaction of conjugated organic hydrocarbons, in particular aromatic species, with metal surfaces has been a major topic in surface science during the past decade. Up to now, the focus has been almost exclusively on alternant hydrocarbons, which are characterized by an even charge distribution and highly delocalized frontier orbitals. In contrast, non-alternant hydrocarbons have uneven charge distributions, which can result in considerable in-plane dipole moments, and more localized frontier orbitals. They also do not obey the Coulson-Rushbrooke pairing theorem and thus have shifted valence levels compared to the isomeric alternant hydrocarbons. In this contribution, we present the first systematic studies of non-alternant aromatic hydrocarbons on the (111) surfaces of Cu, Ag and Au. In particular, we focus on naphthalene as an alternant hydrocarbon and bicyclo[5.3.0]decapentaene (BDP) as its non-alternant counterpart. On the basis of extensive NEXAFS, PES, TPD and STM studies, we show that the non-alternant hydrocarbon interacts much stronger with the metal surfaces, especially in the case of Cu(111), and that the interaction is more localized. The non-alternant species also experiences a considerable out-of-plane deformation, which results from the localization of the frontier orbitals.

O 98.8 Fri 12:15 H24

Layer-resolved evolution of perfluoropentacene thin films on Ag(110) surfaces — •Ebrahim Ghanbari, Markus Aiglinger, Andrea Navarro-Quezada, Thorsten Wagner, and Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria

The optical properties of organic thin films depend on the crystallographic structure and orientation. In addition, the interaction with the substrate can strongly affect electronic and optical properties. Here, we apply polarization dependent differential reflectance spectroscopy (pol-DRS) [1] and photoelectron emission microscopy (PEEM), simultaneously, to study the evolution of perfluoropentacene (PFP) thin films on Ag(110) surface. The adsorption of the organic molecules locally changes photoelectron emission yield of the surface giving rise to the contrast in PEEM. Therefore, PEEM is perfectly suited to study the evolution of the film morphology on the μm scale in real-time whereas, The pol-DRS is employed to investigate the temporal evolution of the (global) optical properties during thin film deposition. The variation of the PEEM and pol-DRS signals during PFP deposition reveal characteristic changes which can be attributed to the completion of subsequent layers and structural phase transition within these layers.

[1] A. Navarro-Quezada, M. Aiglinger, E. Ghanbari, Th. Wagner, and P. Zeppenfeld, *Rev. Sci. Inst.* 86, 113108 (2015)

O 98.9 Fri 12:30 H24

A comparative STM study: adsorption behavior of different benzoporphyrin derivatives on coinage metals — Michael Lepper, Michael Stark, Liang Zhang, 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

A detailed comparative scanning tunneling microscopy (STM) study of the self-assembly of different benzoporphyrin derivatives, among these Ni(II)-5,10,15,20-tetraphenyltetrabenzoporphyrin (NiTPBP) [1], the corresponding free-base analogue 2HTPBP and of Ni(II)-meso-tetrakis (4-tert-butylphenyl) benzoporphyrin (NiTTBPBP) [2], i.e., with additional tert-butyl groups at the para positions of the phenyl substituents on different substrates, namely Ag(111), Cu(111), Cu(110) and Cu(110)-(2x1)O will be presented and discussed. Depending on the actual molecule-substrate combination, the coverage and the sample temperature different adsorption behaviors are observed ranging from polymorphism [1], monomodal supramolecular arrangements [2] to the formation of molecular chains. The results will be interpreted based on the specific molecule-substrate and molecules-molecules interactions [1]. A particular focus will thereby be on the benzo groups which effectively establish a steric hindrance within the porphyrin macrocycle.

[1] M. Lepper et al., J.Phys. Chem. C, 119 (2015) 19897

[2]L. Zhang et al., PCCP, 17 (2015) 13066

O 98.10 Fri 12:45 H24

Self-assembly of triphenylene molecules on the reconstructed Au(111) surface: influence of the surface stacking order — Sören Zint[1], •Daniel Ebeling[1], Sebastian Ahles[2], Hermann A. Wegner[2], and André Schirmeisen[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

Polycyclic aromatic hydrocarbons are an interesting component for the fabrication of nanoscale electronic devices, due to an extended pi-system and the possibility of forming graphene-like material. A powerful tool for the bottom-up fabrication of such nanostructures is molecular self-assembly. We study self-assembly of triphenylene molecules on the reconstructed Au(111) surface at submonolayer coverages by low temperature UHV STM at 5K. The molecules adsorb planarly, in two orientations only, corresponding to a 60° rotation. At low and medium coverages self-assembly is determined by strong attractive surface-molecule interactions and repulsive molecule-molecule interactions, which is accompanied by a one-to-one ratio of molecular orientations. At full monolayer coverage, however, the molecules undergo a reorientation into two different close-packed domains, leading to a significant overrepresentation of one molecular orientation. This reorientation strongly correlates with the stacking order of the substrate. Hence, the self-assembly process is controlled by the interaction of triphenylene with subsurface Au layers, which provides an additional mechanism for designing new systems.

O 98.11 Fri 13:00 H24

Probing the Conformations of Synthetic Sequence Controlled Polymers — Ivan Pentegov[1], Tam Trinh[2], •Stephan Rauschenbach[1], Uta Schlickum[1], Sabine Abb[1], Ludger Harnau[1], Simone Conti[2], Duy Le[3], Talat Rahman[3], Marco Ceccini[2], Jean-Francois Lutz[2], and Klaus Kern[1] — [1]Max-Planck-Institute for Solid State Research, Stuttgart — [2]Université de Strasbourg, France — [3]University of Central Florida, Orlando FL, USA

In natural as well as synthetic sequence controlled polymers (SCP) the sequence of building blocks covalently hardwires a secondary molecular structure, either to store information or to encode properties like molecular conformation. Therefore the two major challenges for the application of SCP are deciphering the sequence of a SCP and relating the sequence to its conformation. We employ scanning tunneling microscopy (STM) to characterize individual SCPs of the class of oligo-triazolamines (OTA) at highest spatial resolution. For this, electrospray ion beam deposition (ES-IBD) ensures chemical purity and intact deposition on ultrapure substrates. We observe conformations, which can be modeled by molecular dynamics (MD) simulations and density functional theory (DFT). Depending on the sequence, we find structural variety depending on the sequence of '0' and '1' represented by the absence or presence of a methyl group, respectively.

O 99: Symposium on Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Time: Friday 9:30–12:15 Location: H1

Invited Talk O 99.1 Fri 9:30 H1
Intrinsic Transport Coefficients and Momentum Space Berry Curvatures — •Allan H MacDonald — University of Texas at Austin, Austin TX, USA

The response of a conductor to a bias voltage is normally dominated by repopulation of states near the Fermi level. The transport steady state is fixed by a competition between acceleration in an electric field and disorder-induced scattering which attempts to restore equilibrium. This response of observables to a bias voltage is therefore extrinsic. There is however also response of states away from the Fermi level, which are polarized by the electric field. Provided that the typical band separation is larger than the finite life-time uncertainty in Bloch state energies this response is intrinsic, and for some observables it can be dominant. Intrinsic response coefficients are attractive targets for electronic structure theory because they are readily evaluated. Examples of responses to bias voltages that are sometimes dominantly intrinsic are the anomalous Hall conductivity of ferromagnetic or antiferromagnetic conductors, the spin-Hall conductivity of heavy metals, and current-induced torques in heavy-metal/ferromagnet systems. Intrinsic transport coefficients tend to be large in crystals with large momentum-space Berry curvatures, for example in crystals with topologically non-trivial electronic structure, and remain finite when a gap opens at the Fermi level to eliminate the Fermi surface. I will discuss some important examples of transport coefficients that are dominated by intrinsic contributions, mentioning as an important case the quantum anomalous Hall effect.

Invited Talk O 99.2 Fri 10:00 H1
Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems — •Jairo Sinova — Johannes Gutenberg Universität Mainz, Staudingerweg 7, 55128 Mainz Germany

As current-driven torques are becoming more relevant in future MRAM technologies, in-plane current magnetization dynamics driven by the so called Rashba spin-orbit torques or through a combination of spin-Hall effect and spin-transfer torque has become more and more important. Understanding these torques is paramount to maximize their use. In recent experiments we have shown that in addition to the intrinsic SHE and STT effect there exists an intrinsic spin-orbit torque originating from the Berry phase of the spin-orbit coupled Bloch electrons analogous to the intrinsic spin Hall effect. This type of torques can be observed through SO-FMR driven experiments. We show this new type of toques in theory and experiments in GaMnAs and show that it can be of similar strength to the strong field-like torque. In addition, we extend these physics to a new type of order-parameter manipulation by currents by examining the combined effect of spin-orbit coupling and anti-ferromagnetic order. We show that in broken inversion symmetry anti-ferromagnets a current will induced a non-equilibrium Néel-order field that will act directly on the Néel order parameter, hence making the direct manipulation of anti-ferromagnets without auxiliary exchange biased coupling to other ferromagnets a new and exciting possibility. One of these type of Néel torques has been recently experimentally confirmed.

Invited Talk O 99.3 Fri 10:30 H1
Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions — •Ewelina Hankiewicz — Wuerzburg University

Topological insulators (TIs) have a bulk energy gap that separates the highest occupied band from the lowest unoccupied band and the metallic gapless states at the edge [1]. Similarly, topological superconductors (TSC) have gapless zero energy states protected by the particle-hole symmetry, which in some cases form Majorana bound states. Here, we focus on the proximity-induced superconductivity in TIs [2] as well as on unusual properties of TSC [3] showing that they both can pave a road to find a Majorana state.

Concerning proximity-induced superconductivity in TIs, we describe a novel superconducting quantum spin-Hall effect, which is protected against elastic backscattering by combined time-reversal and particle-hole symmetry even in magnetic fields [2]. We discuss unusual transport properties of this effect and possible Majorana detection schemes.

Finally, we discuss new systems like TSC on the hexagonal lattices. We develop combined microscopic and macroscopic description of these materials that predicts realistic scanning tunneling microscopy signal in these superconductors [3]. Is there a way to measure Majorana state in these systems?

[1] G. Tkachov and E. M. Hankiewicz, Review in Phys. Status Solidi B 250, 215 (2013). [2] R. Reinthaler, G. Tkachov and E.M. Hankiewicz, Phys. Rev. B 92, 161303(R) (2015). [3] L. Elster, C. Platt, R. Thomale, W. Hanke, and E. M. Hankiewicz, Nature Comm. 6, 8232 (2015).

session break

Invited Talk O 99.4 Fri 11:15 H1
Engineering Topological Quantum States: From 1D to 2D. — •Jelena Klinovaja — University of Basel, Switzerland

I will discuss low-dimensional condensed matter systems, in which topological properties could be engineered per demand. Majorana fermions can emerge in hybrid systems with proximity pairing in which the usually weak Rashba spin-orbit interaction is replaced by magnetic textures. I will discuss candidate materials such as semiconducting nanowires [1] and atomic magnetic chains [2]. One further goal is to go beyond Majorana fermions and to identify systems that can host quasiparticles with more powerful non-Abelian statistics such as parafermions in double wires coupled by crossed Andreev reflections [3,4]. Next, I will focus on 'strip of stripes model' consisting of weakly coupled one-dimensional wires [5-7], where interaction effects in the wires can be treated non-perturbatively via bosonization. Such systems can exhibit the integer or fractional quantum Hall effect, spin Hall effect, and anomalous Hall effect.

[1] J. Klinovaja and D. Loss, Phys. Rev. B 86, 085408 (2012). [2] J. Klinovaja, P. Stano, A. Yazdani, and D. Loss, Phys. Rev. Lett. 111, 186805 (2013). [3] J. Klinovaja and D. Loss, Phys. Rev. B 90, 045118 (2014). [4] J. Klinovaja, A. Yacoby, and D. Loss, Phys. Rev. B 90, 155447 (2014). [5] J. Klinovaja and D. Loss, Phys. Rev. Lett. 111, 196401 (2013); J. Klinovaja and D. Loss, Eur. Phys. J. B 87, 171 (2014). [6] J. Klinovaja and Y. Tserkovnyak, Phys. Rev. B 90, 115426 (2014). [7] J. Klinovaja, Y. Tserkovnyak, and D. Loss, Phys. Rev. B 91, 085426 (2015).

Invited Talk O 99.5 Fri 11:45 H1
Skyrmions – Topological magnetization solitons for future spintronics — •Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Ultrathin magnetic films and heterostructures provide a fantastic playground for the stabilization, manipulation and usage of chiral magnetic skyrmions – topological magnetization solitons – magnetic entities described by a micromagnetic energy functional with particle like properties that may open a new vista for spintronics. A crucial quantity for the chiral skyrmion formation is the Dzyaloshinskii-Moriya interaction (DMI), whose presence in thin films could be established in a concerted effort of first-principles theory and spin-polarized scanning tunneling microscopy. It could be shown that the spin-orbit interaction and the structure inversion-asymmetry in these systems result in a DMI that is strong enough to give rise to one- and two-dimensional lattices of chiral spin-textures, chiral domain walls and even single skyrmions. In retrospect, it is surprising how little is known about the DMI in these metallic systems. In this talk I give insight into the DMI, relating first-principles calculations to different models, discussing the transport properties of electrons *e.g.* the topological (THE) and anomalous (AHE) Hall effect in relation to the spin texture of a skyrmion, and discuss possibilities to tailor the magnetic interactions to enlarge the materials base to stabilize single skyrmions. – I acknowledge fruitful collaborations with D. Crum, J. Bouaziz, B. Dupé, S. Heinze, N. Kiselev, S. Lounis, Y. Mokrousov, A. Nandy, and B. Zimmermann.

O 100: Topological Insulators II

Time: Friday 9:30–12:00 Location: H15

O 100.1 Fri 9:30 H15

Signatures of induced superconductivity in a p-n heterostructure comprised of Sb_2Te_3 and Bi_2Te_3 3D topological insulator thin films with in situ Al capping — •Peter Schüffelgen[1], Daniel Rosenbach[1], Martin Lanius[1], Jörn Kampmeier[1], Gregor Mussler[1], Markus Eschbach[1], Ewa Mlynczak[1], Lukasz Plucinski[1], Martina Luysberg[1], Stefan Trellenkamp[1], Martin Stehno[2], Prosper Ngabonziza[2], Alexander Brinkman[2], Yuan Pang[3], Li Lu[3], Thomas Schäpers[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institut and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]TNW and MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands — [3]Laboratory for Solid State Quantum Information and Computation, Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China

We investigate the transport properties of Sb_2Te_3/Bi_2Te_3 p-n heterostructure topological insulator film-superconductor junctions. The films are grown by means of molecular beam epitaxy on a Si (111) substrate and capped *in-situ* by a thin layer of aluminum to prevent thin film degradation and to preserve the Dirac-like surface states. Josephson junctions are defined by depositing two niobium electrodes, separated by a few tens of nanometers, onto the Sb_2Te_3/Bi_2Te_3 layer. The transport measurements at cryogenic temperatures showed signatures of Andreev reflections and Josephson supercurrents. For wider junctions a Fraunhofer pattern was observed for the critical current, whereas for the narrow junctions a monotonous decrease was found.

O 100.2 Fri 9:45 H15

Teraherz-Induced Chiral Edge Photogalvanic currents in 2D HgTe Topological Insulators — •Kathrin-Maria Dantscher[1], Dimitry A. Kozlov[2], Maria-Theresia Scherr[1], Sebastian Gebert[1], Vasily V. Bel'kov[3], Nikolay N. Mikhailov[2], Sergey A. Dvoretskii[2], Ze Dong Kvon[2], and Sergey D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Institute of Semiconductor Physics, Novosibirsk, Russia — [3]Ioffe Institute, St. Petersburg, Russia

We report on the observation of a chiral photogalvanic current generated in the topological protected edge states of 2D topological insulators fabricated on the basis of 8 nm thick HgTe quantum wells. Illuminating the sample with circularly polarized terahertz radiation and picking-up the signal along the edges we detected a photocurrent whose direction reverses by switching radiation polarization from right- to left-handed one. The influence of the magnetic field, the temperature and the angle of incidence of the radiation to these photocurrents are investigated. We demonstrate that circularly polarized radiation, which, according to selection rules, excites only electrons with a certain spin, results in an imbalance of electron distribution in the k-space and causes a spin polarized electric current.

O 100.3 Fri 10:00 H15

temperature induced shift of the chemical potential of Bi2Te2Se tetradymite topological insulators — •jayita nayak[1], gerhard h fecher[1], siham quardi[1], chandra sekhar[1], claudia felser[1], christian tusche[2], shigenori ueda[3], and eiji ikenaga[4] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]Max Planck Institute of Microstructure Physics, Halle — [3]Synchrotron X-ray Station at SPring-8National Institute for Materials Science, Hyogo 679-5148, Japan — [4]Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, 679-5198, Japan

The temperature dependent HAXPES spectra of Bi2Te2Se reveal the appearance of an additional spectral feature above the band gap at low temperature. It appears at 20 K but is absent in the 300 K spectra and the onset of the main features of the spectra is shifted to lower energies. Momentum resolved photoemission electron microscopy (k-PEEM)was carried out using in order to explain the origin of the additional spectral feature. The measurement provides the evidence of the evolution of bulk bands at low temperature which is caused by the shift of the chemical potential. The bulk sensitive HAXPES valence band spectra are in perfect agreement with first principles calculations.

O 100.4 Fri 10:15 H15

Optical investigation of the three-dimensional Dirac semimetals $CaMnBi_2$ and $SrMnBi_2$ — •Micha B. Schilling[1], Artem V. Pronin[1], Martin Dressel[1], and Youguo Shi[2] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China

The interest in the measurements of optical conductivity in three-dimensional Dirac semimetals is based on the recent theoretical studies [1, 2], where the interband optical response of such systems has been shown to be very peculiar. Namely, the real part of the interband optical conductivity has been predicted to be linear in frequency with the slope being related to the Fermi velocity of Dirac electrons.

We investigated the optical properties of the three-dimensional Dirac semimetals $CaMnBi_2$ and $SrMnBi_2$ by means of Fourier-transform infrared spectroscopy. We measured the reflectivity over a frequency range from 50 to 25000 cm^{-1} at different temperatures down to 10 K and determined the optical conductivity from these measurements. In the presentation, we will discuss our results on the optical conductivity in comparison with theoretical predictions.

[1] P. Hosur, S. A. Parameswaran, and A. Vishwanath, Phys. Rev. Lett. **108**, 046602 (2012). [2] A. Bácsi and A. Virosztek, Phys. Rev. B **87**, 125425 (2013).

30 min. Coffee Break

O 100.5 Fri 11:00 H15

Optoelectronic dynamics in nanocircuits based on the topological insulator Bi2Te2Se — •Mariana Hettich[1], Paul Seifert[1], Christoph Kastl[1], Kristina Vaklinova[2], Marko Burghard[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, D-85748 Garching, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

We report on the optoelectronic dynamics in nanocircuits made of the topological insulator Bi2Te2Se. An on-chip photocurrent pump-probe spectroscopy based on coplanar striplines allows us to identify the different ultrafast photocurrent mechanisms in topological insulators with a picosecond time resolution. We discuss non-equilibrium thermal effects as well as the circular photogalvanic current generation as contributions to the overall photocurrent.

O 100.6 Fri 11:15 H15

Structural Study of Weak Topological Insulator Bi_1Te_1 Films on Si(111) grown by Molecular Beam Epitaxy — •Martin Lanius[1], Markus Eschbach[1], Ewa Mlynczak[1], Jens Kellner[2], Pika Gospodaric[1], Chengwang Niu[1], Elmar Neumann[1], Martina Luysberg[3], Gregor Mussler[1], Lukasz Plucinski[1], Gustav Bihlmayer[1], Stefan Blügel[1], Markus Morgenstern[2], Claus Michael Schneider[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]II. Institute of Physics B and JARA-FIT, RWTH Aachen University, Aachen, Germany — [3]Ernst Ruska-Centre for Microscopy and Spectroskopy with Electrons, Forschungszentrum Jülich, Germany

We have studied the nucleation, growth process and structural composition of the weak topological insulator Bi_1Te_1 on Si(111) substrates by STM and STEM. Bi_1Te_1 is a superlattice of predicted 2D topological insulating materials, one bilayer Bi and two Bi_2Te_3 quintuple layers per unit cell. The van der Waals growth mode of Bi_1Te_1 shows smooth surfaces and a supressed twin domain density. The thin films from several nanometers thickness down to the nucleation regime have been grown by molecular beam epitaxy. STEM measurements of the grown films reveal a high crystalline perfection. Simulations and ARPES measurements show 2D surface states originating from spin-orbit coupling, depending in their structure on the surface termination. Furthermore we will demonstrate the ability to grow n-p heterostructures of n-doped Bi_1Te_1 with the p-doped strong TI Sb_2Te_3.

O 100.7 Fri 11:30 H15

Bi2Se3-based heterostructures including magnetic layers: the case of n-QLs Bi2Se3 ontop of Mn-doped Bi2Se3 — •J. Honolka[1], M. Valiska[2], J. Warmuth[3], M. Michiardi[4], M. Vondracek[1], A. S. Ngankeu[4], V. Holy[2], M. Bianchi[4], G. Springholz[5], V. Sechovsky[2], P. Hofmann[4], and J. Wiebe[3] — [1]Institute of Physics, ASCR, Prague, CZ — [2]Department of Condensed Matter, Charles University, Prague, CZ — [3]INF, University of Hamburg, Hamburg, DE — [4]Department of Physics and Astronomy, iNANO, University of Aarhus, Aarhus, DK — [5]Institute of Semiconductor Physics and Solid Solid State Physics, Johannes-Kepler University, Linz, AT

Interfaces between ferromagnetic and non-magnetic Bi2Se3 phases are studied as a material platform to investigate the influence of spin degrees of freedom on 3D topological insulator (TI) properties.

An inverted geometry of n quintuple layers (QLs) Bi2Se3 ontop of Mn-doped Bi2Se3 is achieved by molecular beam epitaxy for n=0 to n=24 QLs and allows to unhamperedly monitor the development of electronic and topological properties by surface sensitive key techniques like angular resolved photoemission spectroscopy. A gap at the Dirac point is observed at small n, which is gradually filled with increasing n. The Dirac point is fully reestablished at about n = 9 QLs. Band bending effects due to the proximity of the interface with the ferromagnetic layers are discussed.

O 100.8 Fri 11:45 H15

Observation of gapped surface states in the topological regime of the quantum-phase transition in Bi-doped Pb-Sn-Se (111) epitaxial films — •Partha Sarathi Mandal[1], Gunther Springholz[2], Valentyn Volobuev[2], Günther Bauer[2], Evangelos Golias[1], Andrei Varykhalov[1], Jaime Sa'nchez-Barriga[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Institut für Halbleiter und Festkörperphysik, Johannes Kepler Universität, Linz, Austria

Topological crystalline insulators are believed to show a straight forward and versatile connection between mirror symmetries and gap opening at the surface Dirac points. Here we systematically studied the trivial-to-topological insulator phase transition [1] of the $Pb_{1-x}Sn_xSe(111)$ surface grown by molecular beam epitaxy and using angle-resolved photoemission spectorscopy (ARPES) under variation of Sn concentration (10 to 28%) and temperature. Differently from the case of the (001) surface [2], we observe two types of Dirac cones centered at $\overline{\Gamma}$ and $\overline{\mathrm{M}}$ in the surface Brillouin zone. By comparing the band structure of samples with fixed Sn concentration and different Bi doping, we demonstrate the existence of gapped surface states within the topological regime of the quantum-phase transition at low temperatures [1].

[1] Y. Ando and L. Fu Annual Review of Condensed Matter Physics Vol. 6: 361-381 (2015). [2] Y. Tanaka, T. Shoman, K. Nakayama, S. Souma, T. Sato, T. Takahashi, M. Novak, Kouji Segawa, and Yoichi Ando PHYSICAL REVIEW B 88, 235126 (2013).

O 101: Overview Talk: Hans-Peter Steinrück

Time: Friday 13:15–14:00 Location: S054

Invited Talk O 101.1 Fri 13:15 S054

Ionic liquid surface science — •Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg

Ionic liquids (ILs) are molten salts with a melting point below 100 °C. They represent a new class of liquid materials with unique property profiles originating from a complex interplay of Coulombic, hydrogen bonding, and van der Waals interactions of their ions. The enormous variety of cation-anion combinations enables tuning of the physico-chemical properties over a wide range. Functional groups can be implemented in their chemical structure to adapt them for specific tasks - such functionalized ILs are known as 'task-specific ionic liquids'. Applications range from catalysis and organic synthesis to tribology, protective coatings and gate dielectrics. In most cases, the interface of the IL with its environment (gas, liquid, solid) plays an important role. Therefore, knowledge about interface properties and their relation to the chemical structure is of pivotal importance for choosing the right IL for a specific application. In contrast to most other liquids, ionic liquids have a very low vapour pressure, and thus can be studied with the methods of ultrahigh vacuum-based surface science. Thereby, detailed information on their surface composition, on segregation and enrichment effects, on the dissolution and reactivity of catalytically active metal complexes, on the growth of ultrathin IL-layers, and even on reactions in the liquid phase, can be obtained. Many of the derived conclusions are considered representative for liquid surfaces in general.