Surface Science Division
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

(Lecture rooms MA 004 MA 005, MA 041, MA 042, MA 043, MA 141, MA 144, HE 101, HL 001, and HFT-FT 131; Poster A and B)

Invited Talks

O 1.1	Mon	9:30–10:15	HE 101	**Manipulation of Single Functional Molecules: Wires and Motors** — •Leonhard Grill
O 5.1	Mon	10:30–11:00	MA 042	**In-situ studies of organic thin films** — •Thorsten Wagner
O 9.1	Mon	10:30–11:00	HFT-FT 131	**CeO_2(111) defect structure, oxygen migration and polaron hopping: A theoretical perspective** — •M. Veronica Ganduglia-Pirovano, Gustavo E. Murgida, Valeria Ferrari, Ana Maria Llois, Dawei Zhang, Zhong-Kang Han, Yi Gao
O 9.2	Mon	11:00–11:30	HFT-FT 131	**Interactions at the interface between cerium oxide and metals** — •Paola Luches
O 9.3	Mon	11:30–12:00	HFT-FT 131	**Unraveling surface chemistry Of C-H reforming reactions over Ni-CeOx(111) catalysts** — •Sanjaya Senanayake
O 11.1	Mon	15:00–15:30	MA 004	**Elementary phenomena in hybrid graphene nanoribbons on surfaces** — •Nacho Pascual
O 12.7	Mon	16:45–17:15	MA 005	**Nonlinear Surface Phonon Polariton Spectroscopy** — Nikolai C. Passler, Ilya Razdolski, Christopher J. Winta, Sandy Gewinner, Wieland Schöllkopf, Stefan A. Maier, Joshua D. Caldwell, Martin Wolf, •Alexander Paarmann
O 14.1	Mon	15:00–15:30	MA 042	**Non-commensurate epitaxy with and without coincidences** — •Roman Forker
O 14.8	Mon	17:15–17:45	MA 042	**Spotlight on Excitonic Coupling in Textured and Polymorphic Anilino Squaraine Thin Films** — •Manuela Schiek
O 18.1	Mon	15:00–15:30	HE 101	**Surface chemistry of ruthenates** — •Ulrike Diebold, Daniel Halwidl, Wernfried Mayer-Schmözer, Martin Setvin, Florian Mittendorfer, Josef Redinger, Michael Schmid
O 18.2	Mon	15:30–16:00	HE 101	**Multiscale modelling of metal oxide interfaces and nanoparticles** — •Kersti Hermansson
O 22.1	Tue	9:30–10:15	HE 101	**Metal-organic coordination on surfaces: towards complexity and functionality** — •Nian Lin
O 23.1	Tue	10:30–11:00	MA 004	**Electronic properties of functional organic compounds at surfaces: From zero- to two-dimensional** — •Petra Tegeder
O 24.1	Tue	10:30–11:00	MA 005	**Modelling Photo-electrochemistry on Oxide Surfaces** — •Harald Oberhofer
O 24.5	Tue	11:45–12:15	MA 005	**Potential-Specific Structure at the Hematite-Electrolyte Interface** — Martin E. McBriarty, Joanne E. Stubbs, Peter J. Eng, Guido von Rudorff, Jochem Blumberger, •Kevin M. Rosso
O 24.6	Tue	12:15–12:45	MA 005	**Photoelectrochemistry on hematite: a first-principles view** — •Anders Hellman
O 27.1	Tue	10:30–11:00	MA 043	**Inside graphene devices** — •Clemens Winkelmann, Sayanti Samaddar, Alessandro De Cecco, Hervé Courtois, Indra Yudhistira, Shaffique Adam, Vladimir Prudkovskiy, Claire Berger, Walt de Heer

O 30.1	Tue	10:30–11:00	HE 101	**Recent Progress in Nonlinear Phononics and Josephson Plasmonics** — •Andrea Cavalleri
O 30.2	Tue	11:00–11:30	HE 101	**Femtosecond nanoscopy of collective excitations in semiconductors** — •Markus A. Huber, Fabian Mooshammer, Markus Plankl, Leonardo Viti, Fabian Sandner, Miriam S. Vitiello, Tyler L. Cocker, Rupert Huber
O 30.3	Tue	11:30–12:00	HE 101	**Boron nitride nanoresonators for phonon-enhanced molecular vibrational spectroscopy at the strong coupling limit** — •Marta Autore, Peining Li, Irene Dolado, Francisco J. Alfaro-Mozaz, Ruben Esteban, Ainhoa Atxabal, Fèlix Casanova, Luis E. Hueso, Pablo Alonso-González, Javier Aizpurua, Alexey Y. Nikitin, Saül Vélez, Rainer Hillenbrand
O 30.4	Tue	12:00–12:30	HE 101	**Ballistic surface plasmons in high mobility Dirac liquid of graphene** — •Dmitri Basov
O 30.5	Tue	12:30–13:00	HE 101	**Novel Materials and Approaches for Dynamic IR Nano-Optics** — •Joshua Caldwell
O 37.1	Tue	14:00–14:30	MA 141	**Unraveling the structure and dynamics at solid-liquid interfaces by machine learning potentials** — Matti Hellström, Vanessa Quaranta, •Jörg Behler
O 53.1	Wed	9:30–10:15	HE 101	**Elementary steps in surface dynamics and reactivity at electrochemical interfaces** — •Olaf Magnussen
O 54.1	Wed	10:30–11:00	MA 004	**Molecularly functionalized surfaces and interfaces** — •Adam Foster
O 55.8	Wed	12:15–12:45	MA 005	**Growth and surface chemistry of rutile IrO2(110)** — •Jason Weaver
O 57.1	Wed	10:30–11:00	MA 042	**Hydrogen Atom Adsorption on Surfaces Studied in Inelastic Scattering Experiments** — •Oliver Buenermann
O 61.1	Wed	10:30–11:00	HE 101	**Bias-dependent local structure of water molecules at a metallic interface** — •Maria Victoria Fernandez-Serra
O 61.2	Wed	11:00–11:30	HE 101	**Optical imaging of surface chemistry and dynamics in confinement** — •Sylvie Roke
O 61.5	Wed	12:00–12:30	HE 101	**Charge Transfer at the Single Molecule Level with Metal and Semiconductor Electrodes** — •Richard Nichols, Andrea Vezzoli, Richard Brooke, Nicolò Ferri, Simon Higgins, Walther Schwarzacher
O 62.1	Wed	10:30–11:00	HL 001	**Correlating electrons via adiabatic connection approach: a general formalism, approximations, and applications** — •Katarzyna Pernal
O 65.3	Wed	15:30–16:00	MA 005	**Bulk-terminated surfaces of $KTaO_3$ and $SrTiO_3$ studied by combined STM/AFM** — •Martin Setvin
O 67.1	Wed	15:00–15:30	MA 042	**Ultrafast dynamics of two-dimensional electron systems probed by time- and angle-resolved two-photon photoemission** — •Jens Güdde
O 71.3	Wed	15:30–16:00	HE 101	**XPS of ionic liquids: from half-cell to in situ electrochemical measurements** — •Annette Foelske-Schmitz, Markus Sauer, Daniel Weingarth, Rüdiger Kötz
O 71.4	Wed	16:15–16:45	HE 101	**Single-Molecule Switching in 2D Materials at Solid-Liquid Interfaces** — •Stijn F. L. Mertens
O 72.1	Wed	15:00–15:30	HL 001	**Computational Approach to the Electronic Structure of Strongly Correlated Materials: Towards Theoretical Spectroscopy and Theory Assisted Material Design** — •Gabriel Kotliar
O 86.1	Thu	9:30–10:15	HE 101	**Weyl Semimetals and beyond!** — •Claudia Felser
O 87.1	Thu	10:30–11:00	MA 004	**Molecular structures for conductance measurements** — •Richard Berndt
O 88.1	Thu	10:30–11:00	MA 005	**Syngas reactions on metal surfaces studied using scaling-relation-based kinetic Monte Carlo** — •Mie Andersen
O 88.2	Thu	11:00–11:30	MA 005	**Catalytic reactivity of binary alloys studied by field emission techniques** — •Cédric Barroo, Yannick De Decker, Luc Jacobs, Thierry Visart de Bocarmé

O 88.3	Thu	11:30–12:00	MA 005	**Imaging spin polarization and orbital character at surfaces: from the Rashba effect to topological Fermi arcs** — •H. Bentmann, H. Maass, C.-H. Min, F. Reinert
O 88.4	Thu	12:00–12:30	MA 005	**Tuning optoelectronic properties of silicon quantum dots via surface chemistry** — •Mita Dasog, Jonathan G. C. Veinot, Nathan S. Lewis
O 88.5	Thu	12:30–13:00	MA 005	**Carbon Dioxide Activation at Metal-Oxide Surfaces: A Compressed-Sensing Analysis** — •Aliaksei Mazheika, Yanggang Wang, Rosendo Valero, Francesc Illas, Runhai Ouyang, Luca M. Ghiringhelli, Sergey V. Levchenko, Matthias Scheffler
O 92.1	Thu	10:30–11:00	MA 141	**0-D and 1-D heterostructure mediated material properties of 2-D Transition Metal Dichalcogenides** — •Alexander Weber-Bargioni
O 93.1	Thu	10:30–11:00	HE 101	**Ultrafast Electron Diffuse Scattering: Mapping Momentum Dependent Electron-Phonon Coupling and Nonequilibrium Phonon Dynamics in 2D Materials** — •Bradley Siwick, Martin Otto, Laurent Rene de Cotret, Mark Stern, Mark Sutton
O 93.2	Thu	11:00–11:30	HE 101	**Beyond Debye-Waller Effects in Ultrafast Electron Diffraction** — •Xijie Wang
O 100.1	Thu	15:00–15:30	MA 141	**Suitably functionalized molecules on surface: from self-assembly to chemical reactions** — •Shi-Xia Liu, Jascha Repp, Ernst Meyer, Silvio Decurtins
O 101.1	Thu	15:00–15:30	HE 101	**Ultrafast Structural Dynamics in Organic Molecular Solids** — •Heinrich Schwoerer
O 101.2	Thu	15:30–16:00	HE 101	**Ultrafast Electronic Band Gap Control and Self-Protection from a Photoinduced Phase Transition in an Excitonic Insulator** — •Julia Stähler
O 102.1	Thu	15:00–15:30	HL 001	**Recent developments in FCIQMC: real-time propagation and improved convergence with walker number** — •Ali Alavi
O 108.1	Fri	9:30–10:15	HE 101	**Electronic structure of two-dimensional materials revealed by angle-resolved photoemission spectroscopy (ARPES) and Nano-ARPES** — •Shuyun Zhou
O 116.1	Fri	10:30–11:00	HE 101	**Imaging Coherent, Nanoscale Acoustic-Phonon Dynamics with Ultrafast Electron Microscopy** — •David Flannigan, Daniel Cremons, Daniel Du, Dayne Plemmons, Spencer Reisbick
O 121.1	Fri	13:15–14:00	HE 101	**A look through the operando glass: First-principles based multiscale modeling of working catalysts** — •Karsten Reuter

Invited talks of the joint symposium SYID

See SYID for the full program of the symposium.

SYID 1.1	Mon	9:30–10:00	H 0105	**Data driven R&D for Materials: Cognitive Discovery** — •Alessandro Curioni
SYID 1.2	Mon	10:00–10:30	H 0105	**Rational design and synthesis of Pt-based catalysts for fuel cell applications** — •Younan Xia
SYID 1.3	Mon	10:30–11:00	H 0105	**2D, or not 2D? Materials discovery, data provenance, and workflow reproducibility.** — •Nicola Marzari
SYID 1.4	Mon	11:00–11:30	H 0105	**Generating and assessing data from combinatorial and high-throughput experiments for the design of new materials** — •Alfred Ludwig
SYID 1.5	Mon	11:30–12:00	H 0105	**Novel materials discovery: big-data-analytics methods and infrastructure for building maps of materials** — •Luca Ghiringhelli

Invited talks of the joint symposium SYTO

See SYTO for the full program of the symposium.

SYTO 1.1	Wed	9:30–10:00	H 0105	**Beyond Topologically Ordered States: Insights from Entanglement** — •B. Andrei Bernevig
SYTO 1.2	Wed	10:00–10:30	H 0105	**Topological Magnon Materials** — Alexander Mook, Jürgen Henk, •Ingrid Mertig

SYTO 1.3	Wed	10:30–11:00	H 0105	**Topological Order of Interacting Polymers on a Substrate** — •Vincenzo Vitelli
SYTO 1.4	Wed	11:15–11:45	H 0105	**Quantization of Heat Flow in Fractional Quantum Hall States** — •Moty Heiblum
SYTO 1.5	Wed	11:45–12:15	H 0105	**Currents and Phases in Quantum Rings** — •Kathryn Moler

Invited talks of the joint symposium SYTH

See SYTH for the full program of the symposium.

SYTH 1.1	Thu	9:30–10:00	H 0105	**Extracting the electrical properties of metal halide perovskite semiconductors using transient terahertz spectroscopy** — •Michael B. Johnston
SYTH 1.2	Thu	10:00–10:30	H 0105	**THz nanophotonics with 2D materials** — •Miriam SERENA Vitiello
SYTH 1.3	Thu	10:30–11:00	H 0105	**Nonlinear responses and 2D spectroscopy using THz electric and magnetic fields** — •Keith A Nelson
SYTH 1.4	Thu	11:15–11:45	H 0105	**Low energy electrodynamics of correlated spin systems.** — •N. Peter Armitage
SYTH 1.5	Thu	11:45–12:15	H 0105	**Lightwave scanning tunneling microscopy of single molecules** — Dominik Peller, Tyler L. Cocker, Ping Yu, Rupert Huber, •Jascha Repp

Invited talks of the joint symposium SYDM

See SYDM for the full program of the symposium.

SYDM 1.1	Thu	15:00–15:30	H 0105	**Bending, pulling, and cutting wrinkled two-dimensional materials** — •Kirill Bolotin
SYDM 1.2	Thu	15:30–16:00	H 0105	**Ultrafast valley and spin dynamics in single-layer transition metal dichalcogenides** — •Alejandro Molina-Sanchez
SYDM 1.3	Thu	16:00–16:30	H 0105	**Interlayer excitons in layered semiconductor transition metal dichalcogenides** — •Steffen Michaelis de Vasconcellos
SYDM 1.4	Thu	16:45–17:15	H 0105	**Exploring exciton physics in liquid-exfoliated 2D materials** — •Claudia Backes
SYDM 1.5	Thu	17:15–17:45	H 0105	**A Progress Report on Electron Transport in MXenes; A New Family of 2D Materials** — •Michel Barsoum

Invited talks of the joint symposium SYAM

See SYAM for the full program of the symposium.

SYAM 1.1	Fri	9:30–10:00	H 0105	**Bringing Dino-Birds to life – Synchrotron X-ray fluorescence and Raman imaging of ancient materials** — •Uwe Bergmann
SYAM 1.2	Fri	10:00–10:30	H 0105	**Linear and Nonlinear Optical Properties of Cultural Heritage Materials** — •Marta Castillejo
SYAM 1.3	Fri	10:30–11:00	H 0105	**Morphology and topology of multiscale pore networks: Imaging structural alteration and hydric invasion** — •Pierre Levitz
SYAM 1.4	Fri	11:15–11:45	H 0105	**Painting cracks: a way to reveal physical properties of matter** — •Ludovic Pauchard
SYAM 1.5	Fri	11:45–12:15	H 0105	**Finite element analysis and biomechanical interpretation of fossil material properties** — •Emily Rayfield

Sessions

O 1.1–1.1	Mon	9:30–10:15	HE 101	**Overview Talk: Leonhard Grill**
O 2.1–2.10	Mon	10:30–13:00	MA 004	**Scanning probe techniques: Method development I**
O 3.1–3.10	Mon	10:30–13:00	MA 005	**Ultrafast Electron and spin dynamics at interfaces I**
O 4.1–4.9	Mon	10:30–12:45	MA 041	**Plasmonics and nanooptics: Fabrication and characterization**
O 5.1–5.9	Mon	10:30–13:00	MA 042	**Organic-inorganic hybrid systems and organic films I**

O 6.1–6.11	Mon	10:30–13:15	MA 043	**Graphene: Electronic properties, structure and substrate interaction I (joint session O/TT)**
O 7.1–7.10	Mon	10:30–13:00	MA 141	**Heterogeneous Catalysis: Experiment**
O 8.1–8.10	Mon	10:30–13:00	MA 144	**Solid-liquid interfaces: Structure, Spectroscopy I**
O 9.1–9.7	Mon	10:30–13:00	HFT-FT 131	**Focus Session: Frontiers in Reducible Oxide Surface Science I**
O 10.1–10.10	Mon	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)**
O 11.1–11.11	Mon	15:00–18:15	MA 004	**Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures I**
O 12.1–12.11	Mon	15:00–18:15	MA 005	**Ultrafast Electron and spin dynamics at interfaces II**
O 13.1–13.12	Mon	15:00–18:15	MA 041	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy I**
O 14.1–14.10	Mon	15:00–18:15	MA 042	**Organic-inorganic hybrid systems and organic films II**
O 15.1–15.6	Mon	15:00–16:30	MA 043	**Graphen: Adsorption, intercalation and doping I (joint session O/TT)**
O 16.1–16.12	Mon	15:00–18:15	MA 141	**Heterogeneous Catalysis: Theory**
O 17.1–17.6	Mon	15:00–16:30	MA 144	**Solid-liquid interfaces: Reactions and electrochemisty I (joint session O/CPP)**
O 18.1–18.10	Mon	15:00–18:15	HE 101	**Focus Session: Frontiers in Reducible Oxide Surface Science II**
O 19.1–19.9	Mon	15:00–17:15	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)**
O 20.1–20.6	Mon	16:45–18:15	MA 043	**Graphen: Adsorption, intercalation and doping II (joint session O/TT)**
O 21.1–21.6	Mon	16:45–18:15	MA 144	**Solid-liquid interfaces: Reactions and electrochemisty II (joint session O/CPP)**
O 22.1–22.1	Tue	9:30–10:15	HE 101	**Overview Talk: Nian Lin**
O 23.1–23.9	Tue	10:30–13:00	MA 004	**Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures II**
O 24.1–24.8	Tue	10:30–13:15	MA 005	**Focus Session: Structure and Chemistry of Metal-Oxide Surfaces I**
O 25.1–25.10	Tue	10:30–13:00	MA 041	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy II**
O 26.1–26.10	Tue	10:30–13:00	MA 042	**Organic-inorganic hybrid systems and organic films III**
O 27.1–27.10	Tue	10:30–13:15	MA 043	**Graphene: Electronic properties, structure and substrate interaction II (joint session O/TT)**
O 28.1–28.11	Tue	10:30–13:15	MA 141	**Electronic Structure Theory: General I**
O 29.1–29.11	Tue	10:30–13:15	MA 144	**Metallic nanowires on semiconductor surfaces**
O 30.1–30.5	Tue	10:30–13:00	HE 101	**Focus Session: Phonon Polaritons: Opportunities for THz Nanooptics I**
O 31.1–31.5	Tue	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)**
O 32.1–32.6	Tue	14:00–15:30	MA 004	**Electronic structure of surfaces: Spectroscopy, surface states I**
O 33.1–33.5	Tue	14:00–15:15	MA 005	**Semiconductor substrates: Structure, epitaxy and growth**
O 34.1–34.6	Tue	14:00–15:30	MA 041	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy III**
O 35.1–35.7	Tue	14:00–15:45	MA 042	**Organic-inorganic hybrid systems and organic films IV**
O 36.1–36.8	Tue	14:00–16:00	MA 043	**2D materials beyond graphene: TMDCs, silicene and relatives I**
O 37.1–37.7	Tue	14:00–16:15	MA 141	**Electronic-Structure Theory: General II**
O 38.1–38.7	Tue	14:00–15:45	MA 144	**Metal substrates: Adsorption of atoms and inorganic molecules**
O 39.1–39.6	Tue	14:00–15:30	HE 101	**Focus Session: Phonon Polaritons: Opportunities for THz Nanooptics II**
O 40.1–40.2	Tue	15:15–15:45	MA 005	**Semiconductor substrates: Adsorption**

O 41.1–41.7	Tue	18:15–20:30	Poster A	**Poster: Metal Substrates - Structure, Epitaxy, Growth and Adsorption**
O 42.1–42.22	Tue	18:15–20:30	Poster A	**Poster: Organic-Inorganic Hybrid Systems and Organic Films**
O 43.1–43.6	Tue	18:15–20:30	Poster A	**Poster: Semiconductor Substrates - Adsorption**
O 44.1–44.8	Tue	18:15–20:30	Poster A	**Poster: Oxide and Insulator surfaces: Structure, Epitaxy, Growth and Adsorption**
O 45.1–45.21	Tue	18:15–20:30	Poster A	**Poster: Solid-Liquid Interfaces - Structure, Spectroscopy, Reactions and Electrochemistry**
O 46.1–46.5	Tue	18:15–20:30	Poster A	**Poster: Molecular Films - Photovoltaics, Electronics and Morphology**
O 47.1–47.13	Tue	18:15–20:30	Poster A	**Poster: Graphene - Electronic Properties, Structure, Adsorption, Intercalation and Doping (joint session O/TT)**
O 48.1–48.21	Tue	18:15–20:30	Poster A	**Poster: 2D Materials beyond Graphene: TMDCs, Silicene and Relatives**
O 49.1–49.29	Tue	18:15–20:30	Poster A	**Poster: Nanostructures on Surfaces I**
O 50.1–50.7	Tue	18:15–20:30	Poster B	**Poster: Nanostructures on Surfaces II**
O 51.1–51.20	Tue	18:15–20:30	Poster B	**Poster: Electronic Structure of Surfaces: Spectroscopy, Surface States**
O 52.1–52.7	Tue	18:15–20:30	Poster B	**Poster: Electronic structure: Surface Magnetism and Spin Phenomena**
O 53.1–53.1	Wed	9:30–10:15	HE 101	**Overview Talk: Olaf Magnussen**
O 54.1–54.9	Wed	10:30–13:00	MA 004	**Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures III**
O 55.1–55.9	Wed	10:30–13:00	MA 005	**Focus Session: Structure and Chemistry of Metal-Oxide Surfaces II**
O 56.1–56.5	Wed	10:30–11:45	MA 041	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy IV**
O 57.1–57.8	Wed	10:30–12:45	MA 042	**Electronic structure of surfaces: Spectroscopy, surface states II**
O 58.1–58.10	Wed	10:30–13:00	MA 043	**2D materials beyond graphene: TMDCs, silicene and relatives II**
O 59.1–59.10	Wed	10:30–13:00	MA 141	**Nanostructures at surfaces: 1D and 2D structures and networks I**
O 60.1–60.5	Wed	10:30–11:45	MA 144	**Solid-liquid interfaces: Structure, Spectroscopy II**
O 61.1–61.7	Wed	10:30–13:00	HE 101	**Focus Session: Nanoscale Insights into Interfacial Electrochemistry I**
O 62.1–62.9	Wed	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)**
O 63.1–63.4	Wed	12:00–13:00	MA 041	**Plasmonics and nanooptics: Applications and other aspects I**
O 64.1–64.12	Wed	15:00–18:15	MA 004	**Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures IV**
O 65.1–65.6	Wed	15:00–16:45	MA 005	**Focus Session: Structure and Chemistry of Metal-Oxide Surfaces III**
O 66.1–66.10	Wed	15:00–17:45	MA 041	**Plasmonics and nanooptics: Applications and other aspects II**
O 67.1–67.10	Wed	15:00–18:00	MA 042	**Electronic structure of surfaces: Spectroscopy, surface states III**
O 68.1–68.6	Wed	15:00–16:30	MA 043	**Surface dynamics: Reactions, elementary processes and phase transitions I**
O 69.1–69.6	Wed	15:00–16:30	MA 141	**Nanostructures at surfaces: 1D and 2D structures and networks II**
O 70.1–70.5	Wed	15:00–16:15	MA 144	**Solid-liquid interfaces: Reactions and electrochemisty III (joint session O/CPP)**
O 71.1–71.6	Wed	15:00–17:15	HE 101	**Focus Session: Nanoscale Insights into Interfacial Electrochemistry II**
O 72.1–72.10	Wed	15:00–17:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)**

O 73.1–73.5	Wed	16:45–18:00	MA 043	**Surface dynamics: Reactions, elementary processes and phase transitions II**
O 74.1–74.7	Wed	16:45–18:30	MA 141	**Nanostructures at surfaces: Other aspects**
O 75.1–75.5	Wed	16:45–18:00	MA 144	**Solid-liquid interfaces: Reactions and electrochemisty IV (joint session O/CPP)**
O 76.1–76.4	Wed	17:30–18:30	MA 005	**Ultrafast Electron and spin dynamics at interfaces III**
O 77.1–77.26	Wed	18:15–20:30	Poster A	**Poster: Plasmonics and Nanooptics**
O 78.1–78.15	Wed	18:15–20:30	Poster A	**Poster: Surface Dynamics - Reactions, Elementary Processes and Phase Transitions**
O 79.1–79.10	Wed	18:15–20:30	Poster A	**Poster: Ultrafast Electron and Spin Dynamics at Interfaces**
O 80.1–80.20	Wed	18:15–20:30	Poster A	**Poster: Scanning Probe Techniques - Method Development**
O 81.1–81.18	Wed	18:15–20:30	Poster A	**Poster Focus Session: Molecular Nanostructures on Surfaces - New Concepts towards Complex Architectures**
O 82.1–82.15	Wed	18:15–20:30	Poster A	**Poster Focus Session: Frontiers of Electronic-Structure Theory - Correlated Electron Materials**
O 83.1–83.10	Wed	18:15–20:30	Poster A	**Poster Focus Session: Structural Dynamics in Nanoscale Materials, Probed by Ultrafast Electron Pulses**
O 84.1–84.9	Wed	18:15–20:30	Poster A	**Poster Focus Session: Structure and Chemistry of Metal-Oxide Surfaces**
O 85.1–85.9	Wed	18:15–20:30	Poster A	**Poster: Tribology and Misc.**
O 86.1–86.1	Thu	9:30–10:15	HE 101	**Overview Talk: Claudia Felser**
O 87.1–87.9	Thu	10:30–13:00	MA 004	**Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures V**
O 88.1–88.5	Thu	10:30–13:00	MA 005	**Gerhard Ertl Young Investigator Award**
O 89.1–89.10	Thu	10:30–13:00	MA 041	**Oxide and Insulator Surfaces: Structure, Epitaxy and Growth I**
O 90.1–90.10	Thu	10:30–13:00	MA 042	**Electronic structure of surfaces: Spectroscopy, surface states IV**
O 91.1–91.10	Thu	10:30–13:00	MA 043	**2D materials beyond graphene: TMDCs, silicene and relatives III**
O 92.1–92.9	Thu	10:30–13:00	MA 141	**Nanostructures at surfaces: Dots, particles, clusters I**
O 93.1–93.8	Thu	10:30–13:00	HE 101	**Focus Session: Structural Dynamics in Nanoscale Materials, Probed by Ultrafast Electron Pulses I**
O 94.1–94.9	Thu	10:30–12:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)**
O 95.1–95.4	Thu	12:00–13:00	MA 144	**Other And Miscellaneous**
O 96.1–96.12	Thu	15:00–18:15	MA 004	**Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures VI**
O 97.1–97.13	Thu	15:00–18:30	MA 005	**Scanning probe techniques: Method development II**
O 98.1–98.13	Thu	15:00–18:30	MA 042	**Electronic structure: Surface magnetism and spin phenomena I**
O 99.1–99.10	Thu	15:00–17:45	MA 043	**2D materials beyond graphene: TMDCs, silicene and relatives IV**
O 100.1–100.7	Thu	15:00–17:00	MA 141	**Nanostructures at surfaces: Dots, particles, clusters II**
O 101.1–101.7	Thu	15:00–17:30	HE 101	**Focus Session: Structural Dynamics in Nanoscale Materials, Probed by Ultrafast Electron Pulses II**
O 102.1–102.10	Thu	15:00–17:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)**
O 103.1–103.3	Thu	15:45–16:30	MA 041	**Oxide and Insulator Surfaces: Structure, Epitaxy and Growth II**
O 104.1–104.6	Thu	16:45–18:15	MA 041	**Oxides and Insulators: Adsorption I**
O 105.1–105.4	Thu	17:15–18:15	MA 141	**Nanostructures at surfaces: 1D and 2D structures and networks III**
O 106	Thu	19:00–19:30	H 0105	**Annual Meeting of the Surface Science Division**
O 107	Thu	19:30–20:30	H 0105	**Post-Deadline Session**
O 108.1–108.1	Fri	9:30–10:15	HE 101	**Overview Talk: Shuyun Zhou**

O 109.1–109.5	Fri	10:30–11:45	MA 004	**Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures VII**
O 110.1–110.1	Fri	10:30–10:45	MA 005	**New Methods: Theory**
O 111.1–111.8	Fri	10:30–12:30	MA 041	**Oxides and Insulators: Adsorption II**
O 112.1–112.10	Fri	10:30–13:00	MA 042	**Electronic structure: Surface magnetism and spin phenomena II**
O 113.1–113.10	Fri	10:30–13:00	MA 043	**2D materials beyond graphene: TMDCs, silicene and relatives V**
O 114.1–114.4	Fri	10:30–11:30	MA 141	**Nanostructures at surfaces: 1D and 2D structures and networks IV**
O 115.1–115.4	Fri	10:30–11:30	MA 144	**Molecular films: Photovoltaics, electronics and morphology (joint session O/CPP)**
O 116.1–116.8	Fri	10:30–12:45	HE 101	**Focus Session: Structural Dynamics in Nanoscale Materials, Probed by Ultrafast Electron Pulses III**
O 117.1–117.9	Fri	10:30–12:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)**
O 118.1–118.8	Fri	11:00–13:00	MA 005	**Metal substrates: Structure, epitaxy and growth**
O 119.1–119.6	Fri	11:30–13:00	MA 141	**Non-Equilibrium Daynamics in Light-Driven Materials: Theory Meets Experiment**
O 120.1–120.6	Fri	11:30–13:00	MA 144	**Tribology: Surfaces and nanostructures**
O 121.1–121.1	Fri	13:15–14:00	HE 101	**Overview Talk: Karsten Reuter**

Annual General Meeting of the Surface Science Division

Thursday 19:00–19:30 H 0105

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

O 1: Overview Talk: Leonhard Grill

Time: Monday 9:30–10:15 Location: HE 101

Invited Talk O 1.1 Mon 9:30 HE 101
Manipulation of Single Functional Molecules: Wires and Motors — •Leonhard Grill — University of Graz, Department of Physical Chemistry, Heinrichstrasse 28, Graz, Austria

Scanning tunneling microscopy can image surfaces and adsorbed molecules with very high spatial resolution, but is also a powerful tool to manipulate single atoms or molecules. In this presentation recent results with two classes of functional molecules will be discussed: molecular wires for charge transport and molecular motors that cause lateral motion across a surface.

Specifically designed molecular building blocks are connected by on-surface synthesis [1] to one-dimensional chains. When pulling such a single molecular wire off the surface, its electrical [2] and mechanical [3] properties are determined in a highly controlled fashion. Examples of molecular wires with donor and acceptor units [2] or molecular nodes that exhibit different conjugation pathways [4] will be discussed. Molecules were also studied in view of fast lateral motion that could be achieved by specific side groups and an improved manipulation protocol [5]. Moreover, molecules with an internal motor were illuminated by light. Enhanced diffusion across the surface and its wavelength-sensitivity can be directly assigned to the motor unit [6].

[1] L. Lafferentz et al., Nature Chem. 4 (2012) 215, [2] C. Nacci et al., Nature Comm. 6 (2015) 7397, [3] S. Kawai et al., PNAS 111 (2014) 3968, [4] C. Nacci et al., Angew. Chem. Int. Ed. 55 (2016) 13724, [5] G. J. Simpson et al., Nature Nanotech. 12 (2017) 604, [6] A. Saywell et al., ACS Nano 10 (2016) 10945.

O 2: Scanning probe techniques: Method development I

Time: Monday 10:30–13:00 Location: MA 004

O 2.1 Mon 10:30 MA 004
Near-field driven nonlinear photoemission from the tunnel junction of a Scanning Tunneling Microscope — •Benjamin Schröder, Katharina Kaiser, Thomas Kotzott, Murat Sivis, Claus Ropers, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

Scanning Tunnelling Microscopy (STM) is a vital tool for surface chemistry: It gives access to the molecular configuration and the highly site-specific dependencies of chemical reactions. Furthermore, it can drive chemical reactions of individual molecules by applying static fields or injecting electrons by the tunnel current. A desirable extension is the excitation by strongly localized light fields providing intensities that are suitable to trigger nonlinear optical processes.
Here, we present the combination of an ultra-high vacuum low-temperature STM with a femtosecond laser oscillator. The strongly confined optical near-field at the apex is generated by using plasmonic gold nanotips as tunnelling probes. As a demonstration of the field localization, we drive multiphoton photoemission from the tunnel junction under STM operation. The unique capability of the STM to control the tip-sample distance on a sub-Ångström scale allows for the disentanglement of tunnel- vs. photocurrent. We show that the photocurrent gives a topographic contrast of nanometer-scaled surface features.
This project is financially supported by the DFG in the SFB 1073 (project C4).

O 2.2 Mon 10:45 MA 004
A multiprobe scanning tunneling microscope with picosecond time resolution — •Jonas Harm, Johannes Friedlein, Jonas Koch, Maciej Bazarnik, Stefan Krause, and Roland Wiesendanger — Department of Physics, University of Hamburg, Jungiusstraße 11A, 20355 Hamburg, Germany

Here we present a novel design of a 3-tip multiprobe scanning tunneling microscope (MP-STM), which has a picosecond time resolution through the use of RF technology. The microscope consists of two lateral scanners, whose probes are mainly used to contact the sample surface and a central scanner for scanning tunneling microscopy (STM). All three scanners are optimized for their temporal resolution and vibration stability. Using two probes local surface currents can be generated and their effects onto magnetic nanostructures can be investigated on the atomic scale using the central probe tip for spin-polarized STM (SP-STM). Furthermore, the instrument is designed to operate at low temperatures down to 1.5 K and magnetic fields of up to 3 T under UHV conditions. Core concepts of traditional scanning tunneling microscope designs have been combined with novel approaches, such as the use of coaxial RF cabling and connectors. The design concept and first performance tests of the setup under ambient conditions will be presented.

O 2.3 Mon 11:00 MA 004
Influence of microwave radiation on an STM Josephson junction — •Olof Peters[1], Nils Bogdanoff[1], Gaël Reecht[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Univ. Grenoble Alpes, Institut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

Besides its applications in quantum mechanical circuits the Josephson effect is a powerful tool to study the superconducting ground state. The combination of a Josephson junction with the atomic-scale precision of a scanning tunnelling microscope (STM) would enable the measurement of the superconducting order parameter around single magnetic defects. We present here a current-biased Josephson junction in an STM at $T = 1.3\,\mathrm{K}$. Both tip and sample consist of Pb.

Extending the setup with coaxial cables suitable for microwaves makes it possible to couple radiation up to $f = 26\,\mathrm{GHz}$ into the junction where the tip acts as an antenna. The Josephson current responds to the incident microwave radiation by showing multiple steps, with the step position and width depending on the amplitude and the frequency of the microwave radiation. Simulations of the step spacing reveal, that the current is dominated by Cooper pair tunnelling. The power dependence of the steps suggests that the Cooper pair tunnelling is a photon-assisted incoherent process similar as seen by [1].
[1] A. Roychowdhury *et al.*, Phys. Rev. Applied **4**, 034011 (2015)

O 2.4 Mon 11:15 MA 004
Setup of a THz-STM for pump-probe experiments using a commercial THz-source — •Philip Kapitza, Hüseyin Azazoglu, Christian Bobisch, and Rolf Möller — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

To study the excitations of single atoms or molecules on their intrinsic timescales ultrafast temporal and atomic-scale spatial resolution is essential. This can be achieved by combining the very high spatial resolution of a scanning tunneling microscope (STM) with picosecond duration terahertz (THz) pulses. When coupled to the tip of a STM the THz pulses can modulate the bias voltage in the tunneling junction [1,2,3].

The setup presented in this talk consists of a homebuilt low-temperature STM (LT-STM) and a commercial THz-pulse source for time domain spectroscopy (THz-TDS). The THz-emitter of this THz-TDS system is a photoconducting antenna irradiated by a fs-IR laser.

A laser diode is used for the adjustment and focus of the terahertz beam onto the STM tip. First measurements of the time-dependent tunnel current response as well as possible setup for pump-probe-experiments using two terahertz emitters will be presented.

[1] Cocker, T. L. et al., Nat. Photon. 7, 620-625 (2013).

[2] Cocker, T. L. et al., Nature 539, 263-267 (2016).

[3] Yoshioka, K. et al., Nat. Photon. 10, 762-765 (2016)

O 2.5 Mon 11:30 MA 004
Iso-dI/dV - Imaging isodensity contours of molecular states with STM — •Gaël Reecht[1], Benjamin W. Heinrich[1], Hervé Bulou[2], Fabrice Scheurer[2], Laurent Limot[2], and Guillaume Schull[2] — [1]Freie Universität Berlin , Berlin ,Germany — [2]IPCMS,

Strasbourg, France

One of the reason for the success of the Scanning Tunneling Microscopy is the ability to probe the density of states (DOS) of nanostructures adsorbed on surfaces with atomic precision. For mapping the spatial distribution of the DOS, usually constant current or constant height scanning mode is used. Here, we present an alternative method for imaging the DOS of a sample with STM, which consists in mapping the surface topography while keeping the differential conductance (dI/dV) constant [1]. We employ this method, we call iso-dI/dV mapping, to explore archetypical C_{60} molecules on Cu(111). While conventional constant current and constant height mapping methods fail to correctly reproduce the spatial distribution for several orbitals of the C_{60}, the iso-dI/dV maps are in excellent agreement with theoretical simulations of the isodensity contours of the molecular orbitals. Moreover, a direct visualization and unambiguous identification of superatomic C_{60} orbitals and their hybridization is possible.

[1] Reecht et al., New J. Phys., 19, 113033 (2017)

O 2.6 Mon 11:45 MA 004

Resolving Dynamic Processes in Real Space with Variable-Temperature High-Speed Scanning Tunneling Microscopy — •Leonard Gura, Zechao Yang, Patrik Marschalik, Heinz Junkes, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Scanning Tunneling Microscopy (STM) atomically resolved 2D-silica in both, the amorphous [1] and the crystalline state, leading to a structural comparison of the two phases [2]. Resolving dynamic changes in 2D network structures can give indications for the fundamental processes at the atomic scale occurring during glass-transformation.

With the scope of monitoring dynamic processes during the temperature induced change of the network structure, we design a variable temperature high-speed STM. A temperature ramp from 4 to 1500 K is enabled by a continuous-flow cryostat and a sample stage heated by electron bombardment. Thermal drift is reduced due to the symmetric setup of the microscope. For higher frame rates, a spiral scan geometry will be applied, which represents a monotonic continuous function of the angle for the radius without points of inflection nor crossing of lines. The scan is realized with a combination of a conventional STM control unit and custom made high-speed electronics. Due to the high data throughput, programs are needed, which automatically detect atom and ring-center positions in the recorded STM images.

We hope to clarify important structural steps in oxide network structures at so far with STM unrivaled time scales.

[1] DOI: 10.1002/anie.201107097 [2] DOI: 10.1021/jp3062866

O 2.7 Mon 12:00 MA 004

Analysis of the image contrast on Cu(111) using low temperature atomic force microscopy with CO functionalized tips — •Jalmar Tschakert[1], Jannis Jung[2], Tobias Schlöder[2], Olena Lenchuk[2], Doreen Mollenhauer[2], Andre Schirmeisen[1], and Daniel Ebeling[1] — [1]Insitute of Applied Physics, Justus-Liebig-University Giessen, Germany — [2]Insitute of Physical Chemistry, Justus-Liebig-University Giessen, Germany

Low temperature atomic force microscopy with CO-functionalized tips allows to image surfaces and single adsorbed molecules with atomic resolution. Therefore, this so-called bond imaging technique is particularly interesting for studying on-surface catalytic reactions, since it allows to determine molecular adsorption geometries and specific adsorption sites. However, due to the flexibility of the CO tip and different types of short range interactions between the CO tip and the imaged atoms the resulting image contrast is rather complex. When imaging a flat Cu(111) surface this leads to contrast inversions for certain tip-sample distances, which makes it difficult to unambiguously identify atomic sites. To unravel the mechanism behind the contrast formation on Cu(111) we are performing 3D force-field spectroscopy measurements. Therewith, we are able to determine the lateral movement/tilting of the CO molecule and unambiguously identify different atomic sites.

O 2.8 Mon 12:15 MA 004

COFI characterization and imaging of graphene with O-terminated Cu tips — •Alexander Liebig, Daniel Meuer, Angelo Peronio, and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, Germany

The use of chemically inert tips allows to directly probe the repulsive interaction regime and thus to obtain high spatial resolution. Gross et al. found in 2009 [1] that CO terminated metal tips enable intramolecular resolution imaging of organic molecules. Later, it was found that terminating the tip apex with noble gas atoms [2] achieves a similar spatial resolution. Recently, Mönig et al. [3] proposed to use oxygen terminated Cu tips that apparently are also quite inert, but are stiffer in lateral directions than CO tips. To further characterize such O-terminated tips, we apply the COFI method [4], where a CO molecule adsorbed on the Cu surface is used to probe the tip apex. With COFI we are able to resolve the atomic structure of the tip apex. We then use a CuO tip that was characterized with COFI to measure on a graphene monolayer grown on SiC. AFM images of graphene recorded with CO-terminated tips show a deformation of the graphene honeycomb lattice due to the flexibility of the tip apex [5]. We find that for close distances we also see a deformation of the graphene lattice when measuring with an O-terminated Cu tip.

[1] L. Gross et al., Science, 325 (2009) 1110. [2] F. Mohn et al., Appl. Phys. Lett., 102 (2013) 073109. [3] H. Mönig et al., ACS Nano, 10 (2016) 1201. [4] J. Welker, F.J. Giessibl, Science, 336 (2012) 6080. [5] M.P. Boneschanscher et al., ACS Nano, 6 (2012) 10216.

O 2.9 Mon 12:30 MA 004

Compensation method using electrostatic cantilever excitation in electrochemical strain microscopy — •Sebastian Badur, Valon Lushta, Thomas Göddenhenrich, and André Schirmeisen — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392

In contact resonance atomic force microscopy such as electrochemical strain microscopy or piezoresponse, the local tip to sample interaction is superimposed by global electrostatic cantilever excitation due to the cantilever capacitance. Especially when using soft cantilevers, topography and mechanical coupling between tip and sample leads to a significant contribution to the electromechanical imaging signal. On the other hand, one can excite the cantilever in a low and high frequency electric field regime to investigate the latter influence. The cantilever resonance response was measured and analyzed by using the band excitation method on the first contact eigenmode. Measurements are performed under UHV condition using cantilevers with electrical conductive diamond tips.

First results on a $LiNi_{0.5}Mn_{1.5}O_4$ substrate show that with this method we can compensate electrostatic and mechanical crosstalk. This paves the way to obtain true quantitative information about the Vegard strain, which is important for the analysis of ionic movement in battery electrode materials.

O 2.10 Mon 12:45 MA 004

Probing the quantum nature of protons in water with STM/S — •Jing Guo[1], Jinbo Peng[1], Xinzheng Li[2,3], En-Ge Wang[1,3], and Ying Jiang[1,3] — [1]International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, P. R. China — [2]School of Physics, Peking University, Beijing 100871, P. R. China — [3]Collaborative Innovation Center of Quantum Matter, Beijing 100871, P. R. China

Quantum behaviors of protons in terms of tunneling and zero-point motion have significant effects on the macroscopic properties, structure, and dynamics of water even at room temperature or higher. In spite of tremendous theoretical and experimental efforts, accurate and quantitative description of the nuclear quantum effects (NQEs) is still challenging. The main difficulty lies in that the NQEs are extremely susceptible to the structural inhomogeneity and local environments, especially when interfacial systems are concerned. In this talk, I will highlight the recent advances of scanning tunneling microscopy and spectroscopy (STM/S), which allows the access to the quantum degree of freedom of protons both in real and energy space. Then I will discuss how the STM/S are used to directly visualize the concerted quantum tunneling of protons within the water clusters and quantify the impact of zero-point motion on the strength of a single hydrogen bond (H bond) at a water/solid interface. Those results may open up the new possibility of exploring the exotic quantum states of light nuclei at surfaces, as well as the quantum coupling between the electrons and nuclei.

O 3: Ultrafast Electron and spin dynamics at interfaces I

Time: Monday 10:30–13:00 Location: MA 005

O 3.1 Mon 10:30 MA 005

Mechanism of spin-dependent electron transfer on ferromagnetic interfaces: theory and application — •Simiam Ghan, Harald Oberhofer, and Karsten Reuter — Technical University of Munich, Garching, Germany.

Self-assembled monolayers of organic molecules (SAMs) on surfaces show great promise in the emerging field of molecular electronics due to tunable charge transport properties, long-range 2-dimensional order and ease of manufacture. Growth of SAMs on ferromagnetic surfaces offers the additional possibility of spin-dependent transport, making these systems relevant to molecular spintronics in e.g. spin-valves and magnetic tunneling junctions. In order to establish design principles for such applications, a thorough understanding of charge transport mechanisms over SAM-metal interfaces is of great importance.

As an initial benchmark in this direction, we report calculations of spin-dependent electron transport in model systems of Argon monolayers on ferromagnetic Fe(110), Co(0001) and Ni(111) substrates. Spin-polarized charge transfer rates are calculated from the Fermi Golden Rule and explicit time propagation using first-principles parametrized model Hamiltonians. Results are compared to ultrafast core-hole-clock spectroscopy measurements, which found faster transport for minority electrons [1]. After benchmarking the protocol on Ar-metal systems we apply it to thiol-based model SAMs with an aim towards predicting tunable spin-transport behavior.

[1] F. Blobner *et al.*, Phys. Rev. Lett. **112**, 086801 (2014).

O 3.2 Mon 10:45 MA 005

Time-evolution of optical excitations in Fe/MgO(001) heterostructures from RT-TDDFT — •Markus Ernst Gruner, Okan Köksal, and Rossitza Pentcheva — Faculty of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen

We investigate the real-time (RT) evolution of an optical excitation in a $(\mathrm{Fe})_n/(\mathrm{MgO})_m(001)$ multilayer system in the framework of time-dependent density functional theory (TDDFT). The calculations are carried out with the ELK code using the adiabatic local spin density approximation for exchange and correlation. Starting with a minimum model consisting of a single Fe layer and 3 MgO layers, we vary systematically frequency and fluence of the laser pulse and analyse the time dependent propagation of excitations in terms of the variation of the charge density and electronic density of states, which gives insight into the evolution of orbital polarisation. Apart from laser frequency and intensity, we find that also the polarization of light significantly influences the magnitude and propagation of the excitations. First trends for larger systems are discussed.

Financial support from the DFG within SFB 1242 (project C02) is gratefully acknowledged.

O 3.3 Mon 11:00 MA 005

Femtosecond spin-dependent charge transfer at Co/Cu(001) interfaces — •Andrea Eschenlohr[1], Jinghao Chen[1], Tristan Müller[2], Peter Elliott[2], Eberhard K. U. Gross[2], Uwe Bovensiepen[1], and Sangeeta Sharma[2] — [1]Faculty of Physics, University of Duisburg-Essen — [2]Theory Department, MPI for Microstructure Physics, Halle (Saale)

The elementary processes behind ultrafast spin transfer at epitaxial Co/Cu(001) interfaces due to optical excitation with 1.5 eV photon energy are disentangled by combining femtosecond time-resolved interface-sensitive magnetization-induced second harmonic generation and ab initio time-dependent density functional theory. We obtain a convincing agreement between the observables in theory and experiment, which allows us to directly identify spin-dependent charge transfer between Co and Cu active at < 30 fs, and spin-flips mediated by the spin-orbit interaction, which lead to a loss of spatially integrated spin polarization and dominate at > 30 fs. In particular, we find that the charge transfer from Cu into Co is also spin polarized.

We acknowledge funding from DFG through SPP 1840 QUTIF.

O 3.4 Mon 11:15 MA 005

Signature of electron-boson coupling in the non-equilibrium electron population of a Fe-based High-T_c superconductor — •Isabella Avigo[1], Setti Thirupathaiah[1], Manuel Ligges[1], Thomas Wolf[2], Jörg Fink[3], and Uwe Bovensiepen[1] — [1]Universität Duisburg Essen, Fakultät für Physik, 47057 Duisburg, Germany — [2]Karlsruhe Institute of Technology, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [3]IFW-Dresden, Institute for Solid State Research, 01171 Dresden, Germany

Understanding the origin of microscopic interactions among the various electronic, phononic, magnetic degrees of freedom of complex materials, such as High-T_c superconductors, is an essential problem in modern solid state physics. A promising approach is the study of non-equilibrium states and their relaxation in the time domain, as specific coupling channels leave their characteristic fingerprints on the energy-resolved relaxation of the excited electronic population. We present a time-resolved photoelectron spectroscopy (trARPES) study conducted on a Fe-based High-T_c superconductor, where the energy-dependent relaxation rates of the excited electronic population show a characteristic step-behavior around the energy of 200 meV above the Fermi level, indicating the coupling of the excited electronic system to a bosonic excitation, to which we assign a magnetic origin. Our findings further confirm and generalize our previous results obtained on a Cu-based High-T_c superconductor. We acknowledge funding from the DFG through the priority program SPP1458 and the EU within the seventh Framework Program under Grant No. 280555 (GO FAST).

O 3.5 Mon 11:30 MA 005

Femtosecond time-resolved and element-specific x-ray absorption spectroscopy of Fe/MgO — •Nico Rothenbach[1], Andrea Eschenlohr[1], Katharina Ollefs[1], Carolin Schmitz-Antoniak[2], Soma Salamon[1], Rolf Mitzner[3], Niko Pontius[3], Uwe Bovensiepen[1], and Heiko Wende[1] — [1]University of Duisburg-Essen and CENIDE — [2]Forschungszentrum Jülich GmbH — [3]Helmholtz-Zentrum Berlin

A localized optical excitation of a metal/insulator heterostructure induces ultrafast dynamics in its individual compounds, which can involve charge and spin transfer processes as well as coupling to low energy excitations mediated by e.g. electron-electron and electron-phonon scattering. Femtosecond soft x-ray spectroscopy facilitates to separate and identify these electronic and lattice excitations directly in the time domain and, furthermore, is sensitive to the dynamics of the individual constituents itself due to its element-specific character. We have measured time- and element-resolved x-ray absorption spectroscopy of a $[2\,\mathrm{nm}\,\mathrm{Fe}/2\,\mathrm{nm}\,\mathrm{MgO}]_8$ multilayer at the Fe L- and O K-edges with a time resolution of 150 fs. After optically exciting locally Fe with a UV laser pulse of 266 nm wavelength we see a clear pump-induced effect at both edges in fs time resolution. The Fe-signal shows an ultrafast 0.5% dropdown of the signal in 240 fs, followed by a recovery on a 1 ps timescale, while O reaches its maximum not until 1 ps. This slower response suggests that the energy transfer from the metal to the insulator is mediated by phonons, or a combined electronic-phononic process rather than by a direct charge transfer excitation.

O 3.6 Mon 11:45 MA 005

Highly efficient end station for space-, time- and spin-resolved photoemission spectroscopy at free electron lasers. — •D. Kutnyakhov[1], F. Pressacco[2], G. Mercurio[2], L. Wenthaus[2], H. Meyer[2], S. Gieschen[2], A. Oelsner[3], C. Tusche[4,5], Y.J. Chen[4,5], D. Vasilyev[6], K. Medjanik[6], G. Brenner[1], S. Dziarzhytski[1], H. Redlin[1], H.J. Elmers[6], G. Schönhense[6], Y. Acremann[7], and W. Wurth[1,2] — [1]DESY, Hamburg, Germany — [2]CFEL, Univ. Hamburg, Germany — [3]Surface Concept GmbH, Mainz, Germany — [4]FZ Jülich GmbH, Germany — [5]Univ. Duisburg-Essen, Germany — [6]Univ. Mainz, Germany — [7]ETH Zürich, Switzerland

High repetition rate XUV and soft X-ray free electron lasers (FELs) such as FLASH at DESY, Hamburg offer unique possibilities for time-resolved photoelectron spectroscopy (TR-PES). To fully exploit these possibilities it is necessary to use very efficient photoelectrons detection schemes. Combining a time of flight momentum microscope with the FEL as a source is ideal for time- and angle-resolved PES and TR-X-ray photoelectron diffraction to study ultrafast electron- and lattice dynamics. The momentum microscope allows simultaneous detection of the entire band structure with unprecedented efficiency in the full surface Brillouin zone with 3.4 Å^{-1} dia. and 4 eV binding energy range or the angular pattern of core level photoelectrons, respectively, for each time step in a pump-probe experiment. Adding the imaging spin detector extends the capability to detect the spin polarized band structure of the material. The set up was commissioned at FLASH and first results will be presented. Funding BMBF 05K16PGB.

O 3.7 Mon 12:00 MA 005

Intra-atomic Delays in Attosecond Time-resolved Solid State Photoemission — Fabian Siek[1], Sergej Neb[1], Peter Bartz[1], Matthias Hensen[1], Christian Strüber[1], Sebastian Fiechter[2], Miquel Torrent-Sucarrat[3,4,5], Vyacheslav M. Silkin[3,4,5], Eugene E. Krasovskii[3,4,5], Nikolay M. Kabachnik[6,7], Stephan Fritzsche[8], Ricardo Díez Muiño[4,9], Pedro M. Echenique[3,4,9], Andrey K. Kazansky[3,4,5], Norbert Müller[1], •Walter Pfeiffer[1], and Ulrich Heinzmann[1] — [1]University of Bielefeld, Germany — [2]Institut für Solare Brennstoffe, Germany — [3]University of the Basque Country, Spain — [4]Donostia International Physics Center, Spain — [5]IKERBASQUE, Basque Foundation for Science, Spain — [6]Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Russia — [7]European XFEL GmbH, Germany — [8]Helmholtz-Institut Jena, Germany — [9]Centro de Física de Materiales, Spain

Attosecond time-resolved photoemission on the semiconductor WSe_2 allows investigating temporal delays from different initial states with unprecedented resolution. The observed delays cannot be attributed to photoelectron propagation in the solid but intra-atomic corrections such as the formation of a centrifugal barrier must be taken into account to match the experimental results. This sheds new light on the fundamental mechanism involved in the photoemission process from solids on the very initial stage of photoelectron emission, i.e. for the very short time window the emitted electron still resides inside the atom from which it is emitted.

O 3.8 Mon 12:15 MA 005

Femtosecond momentum- and energy resolved electron thermalization dynamics in Cu(100) single crystal studied by time-resolved ARPES — •S. Y. Agustsson[1], D. Vasilyev[1], D. Kutnyakhov[2], K. Medjanik[1], S. Babenkov[1], S. Dziarzhytski[2], H. Redlin[2], D. Curcio[3], F. Pressacco[4], C. Tusche[5,6], Y. Chen[5,6], K. Bühlmann[7], Y. Acremann[7], W. Wurth[2,4], J. Demsar[1], G. Schönhense[1], and H. Elmers[1] — [1]Univ. Mainz — [2]DESY Photon Science — [3]Univ. Aarhus, Denmark — [4]Univ. Hamburg, — [5]FZ Jülich — [6]Univ. Duisburg-Essen — [7]ETH Zürich

The understanding of the photoexcited electron-electron and electron-phonon thermalization dynamics in simple metals and their relation to the inter-subsystem (electron-phonon) coupling strength presents a foundation for similar studies in advanced quantum matter. However, despite the three decades of ongoing research, the understanding is still elusive. Here, we present the first time-, energy-, and momentum resolved photoemission studies of carrier dynamics in Cu (100) single crystal. We used a time of flight momentum microscope with the FEL (FLASH at DESY) as a source (55 eV, <100 fs) to track the changes in the electronic distribution function following photoexcitation with <100 fs NIR pulses from a synced high-repetition rate Ti:Sa amplifier. We demonstrate that the intra-band photoexcitation with an s-polarized light results in changes in the electronic distribution function, which is strongly momentum-dependent. Surprisingly, the momentum anisotropy is observed throughout the electron thermalization process.

O 3.9 Mon 12:30 MA 005

Ultrafast electron and spin dynamics in antiferromagnetic rare-earth intermetallics — •Y. W. Windsor[1], C. Nicholson[1], A. Fedorov[2], M. Puppin[1], K. Kummer[3], K. Kliemt[4], C. Krellner[4], C. Schüssler-Langeheine[5], N. Pontius[5], U. Staub[6], M. Wolf[1], R. Ernstorfer[1], D. V. Vyalikh[7], and L. Rettig[1] — [1]Fritz-Haber-Institut (DE) — [2]IFW Dresden (DE) — [3]ESRF (FR) — [4]Goethe-Univ. (DE) — [5]HZB (DE) — [6]PSI (CH) — [7]DIPC (ES)

Antiferromagnets (AFM) promise much faster magnetization dynamics than ferromagnets (FM), and so are promising candidates for future ultrafast spintronic applications. Here we study the ultrafast electron and spin dynamics in RE-Rh2Si2 AFMs (RE is a rare earth), which exhibit an intriguing coupling of bulk AFM order to a FM surface evidenced by a spin-split surface state [1].

Using XUV time-resolved ARPES (trARPES) and time-resolved resonant X-ray diffraction (trRXD), we obtain a comprehensive view of the ultrafast demagnetization of the bulk AFM and the FM surface (following optical excitation). We observe similar dynamics for the two orders (bulk AFM order and FM spin split surface state), indicating a strong coupling between the two. Comparison of the demagnetization timescales for different RE ions suggests a strong influence of the 4f L moment and spin-lattice coupling on demagnetization, similar to studies on RE metals [2]. Finally, we observe a coherent rotation of the entire AFM structure, which can be controlled by laser fluence.

[1] Güttler, Sci.Rep. 6, 24254 (2016)

[2] Wietstruck, PRL 106, 127401 (2011)

O 3.10 Mon 12:45 MA 005

Direct observation of magnetite surface dynamics by Fast Scanning Tunneling Microscopy — Barbara A. J Lechner, Alexander Bourgund, Ueli Heiz, and •Friedrich Esch — Department of Chemistry & Catalysis Research Center, Technical University of Munich, Lichtenbergstr. 4, D-85748 Garching

Magnetite shows a rich surface chemistry and is a well-known particle support in catalysis [1]. While its surface dynamics have been studied extensively with conventional STM and other techniques [1-3], little is known about these surface processes when studied at the atomic scale at elevated temperatures, with the required high temporal resolution. We present results on the Fe3O4(001) surface dynamics taken with a specially developed FastSTM add-on module [4] that boosts the temporal resolution of our commercial STM up to 12 frames/s, demonstrating the potential of this technique: Surface species and defects that appear similar topographically unravel their different dynamic behavior when increasing temperature stepwise (up to 800 K). In particular, we follow the mobility of H adatoms and of domain boundaries, we observe the subsurface diffusion of Fe atoms and their exchange with the bulk and provide additional insight into the high-temperature transition [3]. Furthermore, the surface morphology is studied under reducing or wet conditions, as well as in an oxygen atmosphere.

References [1] G. S. Parkinson, Surf. Sci. Rep. 2016, 71, 272. [2] R. Bliem et al., Angew. Chem. Int. Ed. 2015, 54, 13999. [3] N. C. Bartelt et al., Phys. Rev. B 2013, 88. [4] F. Esch et al., Rev. Sci. Instrum. 2011, 82, 53702 and NFFA project JRA1.

O 4: Plasmonics and nanooptics: Fabrication and characterization

Time: Monday 10:30–12:45 Location: MA 041

O 4.1 Mon 10:30 MA 041

Refractory plasmonics without refractory materials — •Mario Hentschel[1], Gelon Albrecht[1,2], Stefan Kaiser[1,2], and Harald Giessen[1] — [1]4. Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

Refractory plasmonics deals with metallic nanostructures that can withstand high temperatures and intense laser pulses. The common belief was that refractory materials such as TiN are necessary for this purpose. Here we show that refractory plasmonics is possible without refractory materials. We demonstrate that metallic nanostructures which are overcoated with 4 and 40 nm Al_2O_3 (alumina) by an atomic layer deposition process or by thick IC1-200 resist can withstand temperatures of over 800°C and above, depending on the material, at ambient atmospheric conditions. To provide a comprehensive summary, we compare eight different plasmonic materials, namely Ag, Al, Au, Cu, Mg, Ni, Pd, and Pt. Furthermore, we demonstrate that the alumina coating also aids in nonlinear plasmonic applications where these structures can withstand intense laser radiation of over 10 GW/cm^2 at ambient conditions without damage. Thus, it is possible to combine the excellent linear and nonlinear plasmonic properties of commonly used plasmonic materials with material properties that were believed to be only possible with the lossier and less nonlinear refractory materials.

O 4.2 Mon 10:45 MA 041

Tuning the visual appearance of plasmonic metasurfaces by controlled disorder — •Florian Sterl, Thomas Weiss, Nikolai Strohfeldt, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

The optical properties of plasmonic nanoparticle ensembles are not only determined by the particle shape and size, but also depend on the arrangement of the individual nanoantennas. The angle-dependent transmission and reflection characteristics of a rectangular nanoparticle array are strongly influenced by lattice diffraction effects, while these effects are absent in a completely randomized nanoparticle ensemble. By introducing short-range or long-range disorder into a nanoparticle lattice, one can furthermore strongly influence the optical properties.

We attempt to gain a better understanding of the effect of disorder on the bidirectional reflectance distribution function of complex plasmonic metasurfaces through both simulations and experimental characterization. To this end, we treat the nanoantennas as individual dipoles, and simulate the electric field based on dipole-dipole coupling to approximate the optical image one would obtain from nanoantenna arrays with different degrees of disorder. We compare these results to microscope images and spectroscopic measurements on arrays of gold nanoparticles, addressing both the visual image and the angle-dependent characteristics by using a designated back focal plane spectroscopy setup.

O 4.3 Mon 11:00 MA 041

Fabrication and Near-Field Characterization of Plasmonic Slot Waveguides — •Matthias Liebtrau[1], Mike Prämassing[1], Stephan Irsen[2], and Stefan Linden[1] — [1]Physikalisches Institut, Universität Bonn, D-53115 — [2]Research Center caesar, D-53175

Simulations indicate that plasmonic slot waveguides (PSWs) — based on a sub-wavelength dielectric gap engraved in a thin metal film — permit lateral light confinement siginificantly below the diffraction limit while sustaining mode propagation over several microns [1]. Therefore, PSWs are considered to facilitate highly integrated optical nanocircuits, able to defeat decisive limitations of present electronic and photonic devices [2]. By means of focused ion beam (FIB) milling we manage to fabricate PSWs with slot widths down to 30 nm in a 50 nm gold film, thermally evaporated on silica. We present amplitude- and phase-resolved near-field measurements utilizing a scattering-type scanning near-field optical microscope (s-SNOM) in transmission configuration. Combination with a tunable near-infrared laser source allows for spectroscopic analyses. Following [3] we have deduced the effective index and propagation length of the supported plasmon mode as a function of the slot width at telecom wavelengths. Furthermore, we present our recent studies on slot mode propagation through fundamental integrated circuit elements such as 90°-bends and T-splitters, as well as coupling between neighbouring PSWs.

[1] G. Veronis et al., Opt. Lett. 30, 3359–3361 (2005)
[2] J. A. Schuller et al., Nat. Mater. 9, 193–204 (2010)
[3] A. Andryieuski et al., Nano Lett. 14, 3925–3929 (2014)

O 4.4 Mon 11:15 MA 041

An experimental near-field study of subwavelength nanoaperture arrays in freestanding gold films — •Mike Prämassing[1], Stephan Irsen[2], and Stefan Linden[1] — [1]Physikalisches Institut, Universität Bonn, D-53115 — [2]Research Center caesar, D-53175

Periodic nanoaperture arrays in metallic films with a thickness of several tens of nanometers are well known to exhibit extraordinary optical transmission orders of magnitude higher than predicted by standard aperture theory [1]. In contrast, for very thin metal films a suppressed optical transmission has been reported [2]. Both effects can be explained by resonant coupling of the incident light to surface plasmon polaritons (SPPs) via the array. Here, we present a new fabrication approach for nanoaperture hole arrays in freestanding gold films with thicknesses ranging from 20 nm to 80 nm. Optical transmission spectra of our samples reveal extraordinary transmission, as well as suppressed transmission for the thinner films. Furthermore, we utilize electron energy-loss spectroscopy (EELS) and scattering-type scanning near-field optical microscopy (s-SNOM) as two complementary near-field imaging techniques. EELS directly yields full spectroscopic data of the out-of-plane electric field amplitude $|E_z|$. Combining an interferometric transmission s-SNOM setup with a tunable near-infrared laser source allows for amplitude- and phase-resolved spectroscopic data of E_z. In summary, we are able to connect the SPP near-field patterns to the features in the far-field spectra.

[1] Ebbesen et al., Nature 391, 667-669 (1998).
[2] Braun et al., Phys. Rev. Lett. 103, 203901 (2009).

O 4.5 Mon 11:30 MA 041

Synthesis of atomically flat single crystalline gold platelets for plasmonic applications — •Bettina Frank[1], Timothy J. Davis[1,2], Frank-J. Meyer zu Heringdorf[3], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]2School of Physics, University of Melbourne, Australia — [3]Faculty of Physics and Center of Nanointegration Duisburg-Essen, University of Duisburg-Essen, Germany

We introduce two different methods to produce single crystalline gold platelets. First, we electrochemically create atomically flat single crystalline gold platelets of several tens of micrometers thickness. We investigate their morphology and atomic structure by using AFM, LEEM, and TEM. The second method is a phase transition reaction, where gold ions are transferred to an organic phase which under heating forms single crystalline seeds. After several hours of reaction time single crystalline gold platelets with lateral dimensions of several hundred micrometers are the result. These gold platelets are ideal templates to produce nanostructures via focused ion beam milling. Furthermore, we utilize them for plasmonic applications and demonstrate localized and propagating surface plasmons with EELS and PEEM.

O 4.6 Mon 11:45 MA 041

Perfect Gold Nanoantennas — •René Kullock, Xiaofei Wu, Monika Emmerling, and Bert Hecht — NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Gold nanoantennas find a growing interest in the scientific community as they efficiently link localized electrical fields with propagating electromagnetic light waves. Hence, they can be used to optically excite small volumes of e.g. molecules or – the other way around – enhance the light emission due to inelastic electron tunneling inside the antenna gap [1]. Unfortunately, the performance of antennas often varies strongly as the precision of fabrication methods is limited. Although a lot of advances have been made over the years to increase the accuracy [2], most structures in literature look rather potato-shaped than powerpoint-perfect.

Here, we present a method for fabricating perfect gold nanoantennas on transparent glass substrates in 21 easy steps. The antennas consist of two arms, show crystalline facets and their gaps can be tuned to desired dimensions. The fabrication utilizes top-down as well as button-up methods and will be discussed in detail. We believe that these antennas open up the field to plasmonic experiments with atomic precision.

[1] J. Kern et al., Nat Photon 9, 9 (2015)
[2] J.-S. Huang et al., Nat Comm 1, 150 (2010)

O 4.7 Mon 12:00 MA 041

Optimizing Plasmonic Nanorod Antenna-Arrays — •Tino Uhlig[1], Fabian Patrovsky[1], Vera Fiehler[1], Matthias Böhm[1], Susan Derenko[1], Stephan Barth[2], Hagen Bartzsch[2], Peter Frach[2], and Lukas M. Eng[1] — [1]Institute of Applied Physics, TU Dresden, Germany — [2]Fraunhofer FEP, Dresden, Germany

Gold nanorod antenna arrays provide a strong plasmonic field enhancement and a broad spectral tunability, as needed, for example, for label-free biosensing, surface-enhanced Raman spectroscopy, or optical filter design. However, key issues in utilizing these features, are a reliable fabrication of mostly defect-free nanostructure arrays, as well as a thorough understanding and controlled tuning of the associated optical phenomena. In our work here, we extensively study the plasmonic system based on nanorod arrays, as manufactured by electrochemical pore filling of anodized aluminum oxide (AAO) templates. We present a process that greatly improves anodization of sputtered aluminum thin films, hence dramatically reducing the defect density of such nanorod arrays [1]. The improved homogeneity of our samples is the prerequisite for the clear identification and the detailed analysis of the plasmonic features [2]. Lastly, we introduce an elegant method how to transfer these optimized nanorod arrays from the rigid glass substrate onto an elastically bendable, optically transparent polymer film for mechanically tuning the plasmon resonances over a broad range [3].

[1] F. Patrovsky et al., Mater. Res. Express 4, 055010 (2017).
[2] V. Fiehler et al., J. Phys. Chem. C 120, 12178 (2016).
[3] M. Böhm et al., Opt. Mater. Express 7, 1882 (2017).

O 4.8 Mon 12:15 MA 041

Nano-forging of Gold Rods with Light — •Francis

Schuknecht, Christoph Maier, Anastasia Babynina, and Theobald Lohmüller — Ludwig Maximilians Universität München, Deutschland

V-shaped plasmonic nanoantennas display useful properties as building blocks for meta- surfaces and flat optical devices. Yet, the fabrication of such particles is not a simple task. E-beam lithography is widely used, but shows limitations when it comes to the fabrication of very small nanostructures with high crystallinity. The bending and printing of straight nanorods into desired patterns with light has shown to be a valid alternative approach [1].

Here, we discuss the physical processes governing the bending and orientation of gold nanorods with widths between 8 and 50nm and a length of up to 300nm for varying laser intensities. Additionally to the usage of the particle longitudinal surface plasmon resonance, the transverse plasmonic mode is employed for particle manipulation to examine localised heating effects as a function of the nanorod geometry. The understanding, and parameterisation of the nano-forging process represents a first step to the in-situ creation of efficient ultrathin optical devices.

[1] A. Babynina et al.: Bending Gold Nanorods with Light; Nano Lett, 2016 16(10), pp 6485-6490

O 4.9 Mon 12:30 MA 041

Characterization of 2D nearly-hyperuniform colloidal light management structures — •Lutz Mühlenbein[1], Peter M. Piechulla[1], Alexander Sprafke[1], and Ralf B. Wehrspohn[1,2] — [1]FG Mikrostrukturbasiertes Materialdesign, MLU Halle-Wittenberg — [2]Fraunhofer IMWS, Halle

Interfaces defined by the self-organization of colloidal particles to a monolayer on a substrate are promising candidates for cheap and effective light management structures. By controlling the colloidal size distribution and manipulating the interaction potentials between particles and substrate during the deposition process, we strive to produce structures with tailored light scattering properties to fit the specific requirements of a wide range of potential applications, such as thin-film solar cells and LEDs.

We present a method for fabricating large-area nearly-hyperuniform 2D colloidal structures by a self-stabilized immersion process. Furthermore, we develop a simulative description of the microscopic deposition process by a random sequential adsorption (RSA) model that allows for accurate prediction of structural characteristics of the fabricated samples. On the basis of the structure factor we are able to calculate the optical response by simple means and find good agreement with experimental measurements.

O 5: Organic-inorganic hybrid systems and organic films I

Time: Monday 10:30–13:00 Location: MA 042

Invited Talk O 5.1 Mon 10:30 MA 042

In-situ studies of organic thin films — •Thorsten Wagner — Experimental Physics, Johannes Kepler University Linz, Austria

The performance of electronic devices based on organic thin films,. e.g. LEDs, field effect transistors and solar cells, correlates strongly with the crystalline structure and the morphology of the organic layer. To study the transition of ultrathin films from 2D to 3D growth, Photoelectron Emission Microscopy (PEEM) and Differential Reflectance Spectroscopy (DRS) are applied in situ and in real-time during the deposition of the molecules. The PEEM provides local information on the wetting layer and on μm sized crystallites with a lateral resolution in the 100 nm range. In spectroscopic mode, the electronic density of states is accessible like in conventional UPS but with a much better resolution. The application of linear polarized light for the excitation of the photoelectrons makes the PEEM also sensitive to the in-plane orientation of the molecules. DRS compares the reflectivity of the bare surface to the one of the surface after deposition of molecules. Due to the different environment of the molecules in the first, the second, and higher layers, these layers can be easily identified based on their spectral fingerprints. For anisotropic samples, linear polarized light (pol-DRS) can be used to obtain information about the orientation of the molecules. The combination of both techniques, applied synchronized in one experiment, turns out to be a very powerful tool to make a direct correlation of the morphology and the optical properties of the sample. As an example, the deposition of α-sexithiophene on different silver surfaces will be discussed throughout the entire presentation.

O 5.2 Mon 11:00 MA 042

Momentum resolved electronic structure of the endofullerene Sc3N@C80 on Ag(111) — •Christina Schott[1], Norman Haag[1], Johannes Seidel[1], Leah L. Kelly[1], Mirko Cinchetti[2], Benjamin Stadtmüller[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

Single molecular magnets (SMM) are highly promising materials to reduce the lateral dimensions of magnetic data storage units to the molecular limit. Here, we aim to disentangle the electronic coupling of the organic and the spin carrying part of SMMs and metallic surfaces. As model system, we have chosen the endo-fullerenes Sc3N@C80 for which the atomic spin centers are encased by a robust carbon cage. For a bulk-like film of Sc3N@C80 on Ag(111), we combine momentum resolved photoemission and photoemission tomography to assign the emission features of the molecular orbitals to characteristic parts of the SMM, i.e., to the carbon cage or the atomic spin centers. Spectroscopic differences between the bulk-like film and a Sc3N@C80 monolayer film on Ag(111) can hence be directly linked to the electronic coupling of these molecular parts and the surface. Our results will provide novel insight into the coupling mechanism of spin centers of SMM with (ferromagnetic) metal surfaces and how it influences the properties of spin centers.

O 5.3 Mon 11:15 MA 042

Photoemission study of the spin transition of Fe(phen)2(SCN)2 films on Au(111) — Johannes Stöckl[1,2], •Benito Arnoldi[1,2], Juliusz A. Wolny[1], Volker Schünemann[1], Benjamin Stadtmüller[1,2,3], and Martin Aeschlimann[1,2] — [1]Dept. of Physics, University of Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kl, Ger — [2]Research Center OPTIMAS, Erwin-Schrödinger-Str. 46, 67663 Kl, Ger — [3]Graduate School Materials Science in Mainz, Erwin-Schrödinger-Str. 46, 67663 Kl, Ger

Spin-crossover (SCO) complexes are highly desirable materials for next generation molecular spintronic applications since their electrical, magnetic and optical properties can be controlled by an external stimuli like light or temperature. Here we use angle resolved photoemission electron spectroscopy (ARPES) to investigate the valence band structure of thin films of the prototypical SCO complex Fe(phen)2(SCN)2 on Au(111) for the diamagnetic low spin (LS) as well as the paramagnetic high spin (HS) state. We identify the spectroscopic fingerprints of the HS and LS state by direct comparison of the PES data recorded at room temperature as well as at 40K. In the LS state at LT, the intensity and energetic position of the HOMO-peak of the SCO materials is clearly different compared to the HS state at RT. The magnitude of the observed changes, i.e., the size of the energy shift, strongly dependents on the thickness of the film. Crucially, we show that optical excitation with CW as well as fs light sources can be used to restore the spectroscopic signature of the HS state after the temperature induced transition, i.e., to induce the LS-HS transion.

O 5.4 Mon 11:30 MA 042

Novel 2D Spinterface: Co-TPT/T4PT networks on metallic surfaces — •Lu Lyu[1], Benito Arnoldi[1], Sina Mousavion[1], Sebastian Becker[1,2], Johannes Stöckl[1], Maniraj Mahalingam[1], Benjamin Stadtmüller[1,3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern — [2]Department of Chemistry, TU Kaiserslautern — [3]Graduate School Materials Science in Mainz, Kaiserslautern

Metal-organic networks are highly flexible hetero-structures consisting of atoms which are linked by organic molecules. Most interestingly, the lateral hybridization between the metallic centers and the organic linker molecules can mediate an indirect coupling between the metallic centers which can lead to collective spin phenomena in these systems.

Here, we investigated the geometric and spin-dependent electronic properties of various cobalt based metal-organic networks on cobalt and copper surfaces using LEED, LT-STM and spin-resolved ARPES. As linker molecules, we have chosen the organic molecules TPT (2,4,6-triphenyl-1,3,5-triazine) and T4PT (2,4,6-tri(4-phenyl)-1,3,5-triazine). Upon deposition of these molecules on bare Cu(111) and on thin Co film on Cu(111), metal-organic networks instantaneously formed due to the large amount of free surface adatoms. The Cu-TPT network on Cu(111) reveals single atom cavities which can be filled by Co atoms in an additional deposition step. A comparison between our structural and spin-dependent spectroscopic data will allow us to gain insight into the interactions between the metal atoms and the organic molecules in these networks.

O 5.5 Mon 11:45 MA 042

Towards tailoring the electronic structure of ferromagnetic surface alloys by absorption of organic molecules — •Johannes Seidel[1], Dominik Jungkenn[1], Sina Mousavion[1], Markus Franke[2], Leah L. Kelly[1], Lu Lyu[1], Hans-Joachim Elmers[3], Christian Kumpf[2], Mirko Cinchetti[4], Martin Aeschlimann[1], and Benjamin Stadtmüller[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, D-67663 Kaiserslautern — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, D-52425 Jülich — [3]Institut für Physik, Johannes-Gutenberg-Universität Mainz, D-55122 Mainz — [4]Experimentelle Physik VI, Technische Universität Dortmund, D-44221 Dortmund

In this work, we extend our recent investigations [1] of organic adsorbates on surface alloys to the lanthanide-noble metal surface alloy Dy_1Ag_2/Ag(111). This 2D alloy is highly interesting due to the likely existence of a ferromagnetic phase at low sample temperature [2]. We present a detailed characterization of the electronic structure of the bare Dy_1Ag_2/Ag(111) surface alloy by momentum microscopy. The geometric structure is characterized by STM, LEED and NIXSW. We are able to identify Dy-Ag hybrid states and to reveal a significant vertical buckling of the Dy atoms. Upon the adsorption of PTCDA on Dy_1Ag_2, we find a clear change in the band surface of the surface alloy. These findings will be discussed in the light of the geometric modification of Dy_1Ag_2 surface as well as our previous findings for other surface alloys [1]. [1]PRL**117**, 096805(16); [2]Nano Lett. **16**, 4230(16)

O 5.6 Mon 12:00 MA 042

Band Formation at the Tetraazaperopyrene/Au(111) Interface — •Arnulf Stein[1], Benjamin Günther[2], Lutz H. Gade[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg — [2]Anorganisch-Chemisches Institut, Universität Heidelberg

For the performance of organic semiconductor based (opto)electronic devices the properties of organic/inorganic interfaces play a crucial role. A new class of polyheterocyclic aromatics are the 1,3,8,10-tetraazaperopyrenes (TAPPs) which have already shown to be promising organic semiconductors for applications [1-2]. We studied TAPP-derivatives adsorbed on Au(111) using energy- and angle-resolved two-photon photoemission spectroscopy (2PPE). We determined the electronic structure and observed band formation at the TAPP/Au(111) interfaces.

[1] Martens, S. C. *et al.*, Chem. Eur. J. 18, 3498-3509 (2012).

[2] Hahn, L. *et al.*, Chem. Eur. J. 17691-17700 (2015).

O 5.7 Mon 12:15 MA 042

Structural and electronic phase transition at a metal-organic interface — •Patrick Amsalem[1,2], Luca Giovanelli[2], Oliver Hofmann[3], Georg Heimel[1], Ahmed Khalladi[4], Norbert Koch[1,5], Tobias Rüffer[4], Thierry Angot[2], and Jean-Marc Themlin[1] — [1]Humboldt-Universität zu Berlin & IRIS Adlershof — [2]Aix-Marseille Universitê — [3]Graz University of Technology — [4]Technische Universität Chemnitz — [5]Helmholtz-Zentrum Berlin

The performance of hybrid organic-inorganic devices strongly depends on the interface properties such as the organic / electrode interface. In this context, large research efforts have been devoted to understand the phenomena occurring at interfaces formed between large pi-conjugated molecules and metal surfaces. If much progress has been achieved, the effect of the interplay between molecule-metal and intermolecular interaction on the interface electronic properties is not well-documented yet. Here, we address the structural, vibrational and electronic properties of a long-range ordered sub-monolayer film of octachloro zinc-phthalocyanines (ZnPcCl8) adsorbed on Ag(111), which undergo a structural transition consisting mostly in a decrease of the lattice parameters upon gentle annealing (350 K). The vibrational spectra for the two investigated structural phases reveal strong differences in their electronic properties. In addition, monitoring the change in the valence band features allows to correlate the vibrational features with the amount of charge transfer, as well as with the metallic or insulating character of the hybrid interface.

O 5.8 Mon 12:30 MA 042

On-Surface Synthesis of Heptacene and its Interaction with a Metal Surface — •Malte Zugermeier[1], Manuel Gruber[2], Martin Schmid[1], Benedikt P. Klein[1], Lukas Ruppenthal[1], Philipp Müller[1], Ralf Einholz[3], Wolfgang Hieringer[4], Richard Berndt[2], Holger F. Bettinger[3], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [3]Institut für Organische Chemie, Eberhard Karls Universität Tübingen, Germany — [4]Lehrstuhl für Theoretische Chemie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Acenes are important molecular organic semiconductors, whose electronic properties scale with the length of the conjugated system. With increasing length, the HOMO-LUMO gap and the reorganization energy decrease, while the charge carrier mobility increases. These changes, which are potentially beneficial for applications in organic electronics, are accompanied by unfavorable trends such as increased light sensitivity, increased reactivity towards oxygen, and a higher tendency to form dimers. Therefore, the existence of the larger heptacene was controversial for several decades. We report the on-surface synthesis of heptacene from a diketone precursor on Ag(111) and show that heptacene is stabilized by the presence of the surface. The surface-assisted reaction was monitored by XPS and STM. NEXAFS and DFT provide additional insights into the orientation and the surface interaction of the molecules.

O 5.9 Mon 12:45 MA 042

Metal-Phthalocyanines on Noble Metal Surfaces: A Systematic Investigation With Respect to Strong Correlation Effects — •Manuel Grimm, Dennis Hein, Christian Metzger, Martin Graus, Achim Schöll, and Friedrich Reinert — Exp. Physik 7, Universität Würzburg, 97074 Würzburg, Germany

Metal-organic interfaces provide an ideal playground to study fundamental interaction mechanisms. In particular cases, these can lead to electronic correlations which cannot be described within a single particle picture. In case of some adsorbate/substrate combinations the LUMO of molecules in the first layer is partially occupied due to charge transfer from the metal substrate. As a result such samples, e.g. NTCDA or CuPc on Ag(111) [1,2] show a sharp Kondo resonance at the Fermi energy in high resolution photoelectron spectroscopy (PES) experiments. Here we present a systematic study of these resonance features. We analyze the influence of sample temperature and vary the bonding strength and charge transfer at the interface by changing the adsorbate and the orientation of the substrate surface. While we observe a Kondo scenario for NiPc and CuPc on Ag(111) which is explained within a Single Impurity Anderson model (SIAM), a more complicated behavior occurs on Ag(100) and Ag(110) surfaces. In the latter cases the NiPc and CuPc LUMO is still partially filled at room temperature, but starts to shift to larger binding energies upon cooling. This also leads to a shift of the sharp resonance peak away from the Fermi energy, which demands for an explanation beyond the SIAM.

[1] Schoell *Science* 329, 303 (2010) [2] Ziroff *PRB* B85 (2012)

O 6: Graphene: Electronic properties, structure and substrate interaction I (joint session O/TT)

Time: Monday 10:30–13:15 Location: MA 043

O 6.1 Mon 10:30 MA 043

A Molecular Model System for 5-7 Defects in Graphene — •Benedikt P. Klein[1], Markus Franke[2], Claudio K. Krug[1], Stefan R. Kachel[1], Phil Rosenow[1], Francois Posseik[2], Martin Schmid[1], Reinhard J. Maurer[3], Ralf Tonner[1], Christian Kumpf[2], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [3]Department of Chemistry, University of Warwick, United Kingdom

The electronic and mechanical properties of graphene are strongly influenced by the presence of defects. One important type of defect is the 5-7 motif with a 5-membered ring adjacent to a 7-membered ring. Little is known about the interaction of 5-7 defects with an underlying substrate. In this study, we have obtained insight into this interaction by using molecular model systems. As a model for the 5-7 defects we use azulene, which is a bicyclic aromatic compound with a 5- and a 7-membered ring, while naphthalene is used as a model for the regular 6-6 motif. We investigated both molecules on Cu(111) and Ag(111) using PES, NEXAFS, TPD, scanning probe and NIXSW experiments. To deepen the understanding of the occurring interactions between molecule and surface, periodic DFT calculations were performed. The more localized frontier orbitals of azulene result in a much stronger and more localized interaction with the Cu(111) surface. This leads to interfacial charge transfer in the former LUMO and substantial in-plane and out-of-plane deformations, as well as a much smaller adsorption height.

O 6.2 Mon 10:45 MA 043

The Effect of Carbon 1s Core Hole on the Polarization Spectra of HOPG - theory and experiment — •Dominik Legut[1], Christine Jansing[2], Hans-Christoph Mertins[2], Andreas Gaupp[2], Peter M. Oppeneer[3], Heiko Timmers[4], and Hud Wahab[4] — [1]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [2]FH Mnster, Stegerwaldstr. 39, D-48565 Steinfurt, Germany — [3]Dept. of Physics and Astronomy, Box 530, S-751 21 Uppsala, Sweden — [4]Univ. of New South Wales Canberra, Australia

Our band structure calculations show a good agreement with experimental polarization spectra [1] across the carbon 1*s* edge of highly oriented pyrolytic graphite. The change of polarization characteristics upon reflection of linearly polarized synchrotron radiation as the huge rotation of polarization plane of up to 140° and the change to nearly fully circularly polarized light can be resembled good, showing best results for not full but partially core hole per excitation. The contributions from the *A* and *B* site of HOPG are discussed as well as the amount of electron removed from core state.

References: 1. C. Jansing et al, PRB **94**, 045422 (2016).

This work was supported by Czech National Foundation grant No. 17-27790S and Path to Exascale project No. CZ.02.1.01/0.0/0.0 /16_013/0001791.

O 6.3 Mon 11:00 MA 043

Giant magneto-photoelectric effect at a graphene edge — •Friedemann Queisser, Jens Sonntag, Annika Kurzmann, Martin Geller, Sascha Lang, Axel Lorke, and Ralf Schützhold — Fakultät für Physik, Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg, Germany

Graphene is a promising material for optical or infrared absorption, as its pseudo-relativistic energy-momentum relation allows for a broad absorption bandwidth. In [1] we studied the charge separation at a graphene edge via a strong magnetic field. Motivated by the proposed mechanism, a surprisingly high magneto-photocurrent was measured in suspended graphene [2]. The observed photo-responsitivity (100 incident photons create up to 17 particle-hole pairs) strongly exceeds the predicted value. A possible mechanism to explain the large observed current is Auger-type scattering. The strong Coulomb interaction, $\alpha_{\text{graphene}} \gg \alpha_{\text{QED}}$, together with the enlarged phase space at the graphene edge lead to a large probability per unit time for the secondary particle-hole pair creation. We discuss various aspects of Auger-type scattering at the graphene edge.

References:

[1] F. Queisser and R. Schützhold *Phys. Rev. Lett.* **111**, 046601 (2013)

[2] J. Sonntag, A. Kurzmann, M. Geller, F. Queisser, A. Lorke, R. Schützhold, *New. J. Phys.* **19** 063028 (2017)

O 6.4 Mon 11:15 MA 043

Synthesis of two-dimensional materials using liquid metal catalysts: Instrument development for *in situ* studies — •Amirmehdi Saedi[1], Marc de Voogd[2], Arthur Sjardin[2], Gertjan van Baarle[2], and Irene Groot[1] — [1]Catalysis and Surface Chemistry, Leiden Institute of Chemistry, Leiden University, The Netherlands — [2]Leiden Probe Microscopy BV, Leiden, The Netherlands

Two-dimensional materials (2DMs), e.g. graphene, hold great promise for future applications in many technological areas. The current state-of-the-art synthesis method of these materials involves the dissociative adsorption of gas-phase precursors on a solid catalyst. This process is slow by nature, inefficient, and environmentally unfriendly. Using liquid metal catalysts (LMCats) instead of solid ones bears the prospect of a continuous production of 2DMs with unprecedented quality and production speed. The aims of this multinational collaborative project are to develop instrumentation capable of studying the ongoing chemical reactions on a LMCat, *in situ* investigations on its catalytic activity, and unraveling the growth mechanisms of 2DMs on surfaces of LMCats. Gaining this knowledge would be the key toward establishing the first efficient mass production method for 2DMs using this new technology. (Visit http://lmcat.eu/ for more info)

O 6.5 Mon 11:30 MA 043

Effects of bi-axial strain on heterostructure of hBN and graphene — •Francesco Delodovici[1], Silvana Botti[2], and Giovanni Onida[1] — [1]Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy — [2]Institute of Condensed Matter Theory and Optics Max-Wien-Platz 1 07743 Jena Germany

I will present a theoretical/computational study of the mechanical and electric properties of an heterostructure consisting of graphene superimposed to hexagonal boron nitride (hBN) when external biaxial strain is applied.

As a preliminary case, we consider a free-standing layer of hBN under uniform biaxial strain: we predict new thermodinamically stable configurations and analyze their mechanical properties, to understand whether they could be accessible experimentally. In addition, we characterize their electrical and optical properites, to detect the emergence of radical changes in hBN properties.

Further on, we turn our attention to the effects of equi-biaxial strain on the graphene-hBN heterostructure.

We use ab-initio crystal structure prediction, and more precisely the fixed-volume minima hopping method to sample the configuration space searching for new configurations. We use density functional tight binding methods to obtain energies and forces for structural prediction and DFT to characterize the electric properties of the new phases.

O 6.6 Mon 11:45 MA 043

Light-field-driven currents in graphene — •Christian Heide, Takuya Higuchi, Konrad Ullmann, Heiko B. Weber, and Peter Hommelhoff — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Strong-field physics centres on controlling the motion of electrons by virtue of an optical electric field with attosecond (10^{-18} s) precision. Graphene is an ideal playground for extending the scope of strong-field phenomena to a conductor because of its excellent carrier mobility, much weaker screening due to a low carrier concentration compared with conventional metals and its ultrafast and broadband optical response.

We will show that one can control the residual conducting current in epitaxially grown graphene by tailoring the electric-field waveform of few-cycle laser pulses, on attosecond timescales [1]. We interpret the waveform-dependent conducting current by considering graphene as a simple two-band system, interacting with an oscillating optical field of an ultrashort laser pulse. We found a transition from the weak, perturbative nonlinear response (photon-driven) to optical-field-driven, nonperturbative electron dynamics, in which the influence of the intraband dynamics to the interband transition cannot be neglected. Inthis strong-field regime, electrons exhibit quantum-mechanical interference known as Landau-Zener-Stückelberg interference.

[1] T. Higuchi, C. Heide, K. Ullmann, H. B. Weber, and P. Hommelhoff, Light-field-driven currents in graphene, Nature 550, 224 (2017).

O 6.7 Mon 12:00 MA 043

Can the Coulomb interaction be added to the Dirac-Weyl equation of graphene? — •Fabian Rost and Sam Shallcross — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen, Germany

On the basis of an exact operator equivalence between a lattice tight binding model and a continuum description $H(\mathbf{r},\mathbf{p})$ [1], we address the question of the required form the interaction potential $V_{eff}(\mathbf{r},\mathbf{r}')$ should take in the continuum description in order to maintain operator equivalence with the tight-binding Hamiltonian in the presence of an interaction potential $V(\mathbf{r},\mathbf{r}')$. To lowest order we find the natural answer: that $V_{eff}(\mathbf{r},\mathbf{r}') = \mathbf{V}(\mathbf{r},\mathbf{r}')$ but also that this is sufficient only in the case that $V(\mathbf{r},\mathbf{r}')$ does not change on the scale of the lattice constant. Taking the example of graphene we derive the corrections to the lowest order result for the case of the Coulomb interaction.

[1] N. Ray et al., arXiv preprint arXiv:1607.00920, 2016

O 6.8 Mon 12:15 MA 043

Optical deformations in graphene — •Reena Gupta and Sam Shallcross — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany

Deformations in graphene slow on the scale of the lattice constant are, at lowest order, very well described by the addition of a pseudo-magnetic gauge field to the Dirac-Weyl equation [1]. Here we explore what happens when we consider slow deformations but of both possible modes that the two-atom unit cell allows, i.e., optical as well as acoustic modes. While the acoustic mode simply reproduces the well-known pseudo-magnetic gauge field, the optical mode generates both a chiral field as well as an imaginary magnetic gauge, with Hermiticity of the Hamiltonian maintained by a position dependent velocity correction. We comment on the relevance of these results to hybrid metal/graphene systems which feature strong deformation.

[1] B. Amorim et al., Physics Reports 617, 1 (2016).

O 6.9 Mon 12:30 MA 043

Moiré ordered current loops in the graphene twist bilayer — •Dominik Weckbecker and Sam Shallcross — FAU Erlangen-Nürnberg, Institut für Theoretische Physik, Staudtstrasse 7/B2, 91058 Erlangen, Germany

Moiré lattices in layered two dimensional materials possess, in the presence of a magnetic field of 1-5 Tesla, comparable structural and magnetic length scales and, as a consequence, exhibit remarkable magnetic field phenomena such as the recently observed Hofstadter butterfly [1,2].

In this contribution, we present the results of our simulations on twisted bilayer graphene nanoribbons, which were conducted using a semi-empirical tight-binding method [3].

We report novel phenomena arising from this interplay of length scales in the form of an ordered array of permanent current loops throughout a moiré generated by twisting graphene layers [3,4]. Strikingly, these current loops are found at significantly weaker fields than those required to observe the Hofstadter butterfly, and such current loops thus represent an additional low field imprint of the moiré lattice on Landau physics, and an unusual situation in which the field induced currents are found in the bulk of a material.

[1] D. R. Hofstadter, Phys. Rev. B 14, 2239 (1976)
[2] C. R. Dean et al. , Nature 497, 598-602 (2013)
[3] W. Landgraf et al., Phys. Rev. B. 87, 075433 (2013)
[4] manuscript in preparation

O 6.10 Mon 12:45 MA 043

A novel delocalized phase in the small angle graphene twist bilayer — •Maximilian Fleischmann, Reena Gupta, Dominik Weckbecker, and Sam Shallcross — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany

In this work we demonstrate that the small angle limit of the graphene twist bilayer contains, in addition to its well known localized phase [1], a novel delocalized phase accessible by applied interlayer bias. This phase differs profoundly from the large angle delocalized phase as, in contrast to the almost perfectly circular Fermi surface found at large angles, one finds almost perfectly linear Fermi lines. These may be translated into each other by a so-called nesting vector, the magnitude of which is controllable by the applied field. The finding of a phase in the twist bilayer consisting solely of one dimensional Fermi lines connected by field tunable nesting vectors, marks this system out as an unexpected playground for the study of nested Fermiology and electronic instabilities.

[1] D. Weckbecker et al., Phys. Rev. B **93**, 035452, 2016.

O 6.11 Mon 13:00 MA 043

Electronic and geometric structure of PTCDA films adsorbed on Graphene passivated Ni(111) — •Dominik Jungkenn[1], Johannes Seidel[1], Florian Haag[1,2], Leah L. Kelly[1], Mirko Cinchetti[3], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Erwin-Schrödinger-Str 46, 67663 Kaiserslautern — [2]Graduate School of Excellence Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern — [3]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund

Organic molecules are highly intriguing materials for spintronics due to their wide range of functionalities. However, to take full advantage of these functionalities, ferromagnetic surfaces have to be passivated , either by an organic buffer layer or by an inert 2D material [1]. Along these lines, we have investigated the geometric and electronic structure as well as the hot electron dynamics of a PTCDA monolayer on a Graphene (Gr) passivated Ni(111) surface. We find the formation of long-range ordered PTCDA monolayer films on Gr/Ni(111) resembling the herringbone structure of PTCDA/Ag(111). The frontier molecular states reveal the orbital emission pattern of unperturbed PTCDA molecules suggesting, as expected, a weak coupling of the molecular layer to the Graphene sheet. [1] Cinchetti et al. Nat. Mater. 16, 507 (2017)

O 7: Heterogeneous Catalysis: Experiment

Time: Monday 10:30–13:00 Location: MA 141

O 7.1 Mon 10:30 MA 141

Mechanisms in the Photocatalytic Hydrogen Evolution — •Martin Tschurl[1], Constantin Walenta[1], Sebastian Kollmannsberger[1], Carla Courtois[1], Rui Pereira[2], Martin Stutzmann[2], and Ueli Heiz[1] — [1]Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — [2]Walter Schottky Institute and Physics Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

Sustainable energy production and storage is considered one of the major challenges of the future, as the burning of fossil fuels has a severe impact on our climate. One promising technology to meet this challenge is photocatalysis, which is inspired by the idea to use (sun)light for the generation of renewable fuels as e.g. hydrogen. State-of-the-art materials often comprise co-catalyst loaded semiconductors, but these systems are still limited in efficiency. The development of more powerful catalysts may have been hindered by lack of insights on a molecular scale, as the exact mechanistic details are so far surprisingly little understood. In this talk, detailed mechanisms of the hydrogen evolution on a titania model systems are presented and the consequences for the development of future catalyst materials are discussed.

O 7.2 Mon 10:45 MA 141

Temperature Effects in the Photocatalysis of Co-Catalyst Decorated Titania (110) — •Carla Courtois[1], Constantin Walenta[1], Sebastian Kollmannsberger[1], Martin Tschurl[1], Rui Pereira[2], Martin Stutzmann[2], and Ueli Heiz[1] — [1]Chair of

Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — [2]Walter Schottky Institute and Physics Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

In this study, we show the influence of temperature for photocatalytic reactions on an n-type semiconductor surface. The reactions are investigated for different temperatures under very well defined conditions (UHV). The photooxidation mechanisms proceed via a direct hole transfer to the adsorbed molecules. It is found that the outcome of the photochemical reactions is strongly governed by the thermal adsorption/desorption properties of the involved molecules and can be controlled by the judicious choice of the reaction conditions.

O 7.3 Mon 11:00 MA 141

Evolution of the reactivity of gas-phase cationic tantalum-2 oxide clusters with methane — •George Goddard[1,2], Jan Eckhard[1], Tsugunosuke Masubuchi[1], Martin Tschurl[1], and Ueli Heiz[1] — [1]Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — [2]Department of Chemistry, Durham University, Durham, U.K. DH1 3LE

Metal clusters have long been looked at as model catalysts, particularly in the activation of C-H bonds. It is also known that the presence of ligands can have large effects on reactivity. Here the reaction pathway and kinetics of $Ta_2O_x^+$ with methane were investigated for $x =$ 0-6. $Ta_2O_3^+$ purely shows molecular adsorption, as does $Ta_2O_4^+$ and $Ta_2O_6^+$. Conversely, Ta_2O^+ is unreactive, whilst Ta^+ eliminates H_2 to give a carbene adsorbate, and $Ta_2O_2^+$ shows both intact adsorption and dehydrogenated products of methane. Finally the stoichiometric $Ta_2O_5^+$, which occurs with the lowest abundance causes hydrogen atom abstraction. The reaction was repeated using deuterated methane to confirm mass assignments and to calculate the kinetic isotope effect for each reaction step. This has led to an elucidation of the mechanism and of the structure of the clusters in question.

O 7.4 Mon 11:15 MA 141

Methane activation mediated by free tantalum cluster cations: reactivity governed by cluster size — •Tsugunosuke Masubuchi[1], Jan Eckhard[1], George Goddard[1,2], Martin Tschurl[1], Robert Barnett[3], Uzi Landman[3], and Ueli Heiz[1] — [1]Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — [2]Department of Chemistry, Durham University, Durham, U.K. DH1 3LE — [3]School of Physics Georgia Institute of Technology Atlanta, Georgia 30332-0430, U.S.A.

Methane activation, which involves C-H bond cleavage, is an important topic for versatile use of methane as a feedstock. Many efforts have been made to seek efficient C-H activation of methane in the non-scalable size regime. In this contribution, we report the reactivity of size-selected tantalum cluster cations toward methane molecules, which are investigated under multi-collision conditions. Under such conditions cluster ions are thermalized to desired temperatures, adjustable in a wide range, thus advantageous to explore reaction kinetics.

The mass spectrometric approach shows that tantalum clusters with a certain size exhibit hydrogen elimination from methane at room temperature. On the other hand, the number of the dehydrogenated molecules bound to the cluster changes with cluster size. This feature is associated with the formation of dehydrogenated products.

O 7.5 Mon 11:30 MA 141

Operando X-ray absorption study on the influence of Ce^{3+} species on activity of Au/CeO_2 catalysts in the CO oxidation — •Joachim Bansmann, Ali Abel-Mageed, Gabriela Kucerova, Yuchen Wang, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

The catalytic activity and the deactivation behavior of Au/CeO_2 catalysts in the CO oxidation reaction depend strongly on the reductive or oxidative nature of the pretreatment [1]; oxidative pretreatments result in higher reaction rate. Detailed studies led to the following findings: Independent of the initial chemical state of the Au NPs directly after the pretreatments, the Au NPs always assumed a metallic state a few minutes after starting the reaction.

In this project, we investigated a possible influence of the chemical state of the ceria support (the ratio of Ce^{3+} to Ce^{4+} species) on the catalytic activity of Au/CeO_2 catalysts in the CO oxidation reaction by operando XAS measurements at the Ce L_3 edge. Directly after reductive pretreatments, the ceria support has a relatively high fraction of Ce^{3+} species (6-10%), whereas only 1% was found in case of an oxidative pretreatment. Independent of the initial state of the support, the amount of Ce^{3+} species decreased rapidly (within 10 min) during reaction (1%CO, 1%O_2, rest N_2) to values between about 1% or even less (oxidative pretreatment). Higher values are only observed in CO rich gas mixtures. These findings are discussed with respect to activity of the catalyst and the chemical state of the Au NPs.

[1] A. Abd-El Moemen et al., J. Catal. 341 (2016) 160

O 7.6 Mon 11:45 MA 141

Segregation Phenomena in Size-Selected Bimetallic CuNi Nanoparticle Catalysts — •Lukas Pielsticker[1], Ioannis Zegkinoglou[1], Nuria J. Divins[1], and Beatriz Roldan Cuenya[1,2] — [1]Department of Physics, Ruhr University Bochum — [2]Department of Interface Science, Fritz-Haber Institute of the Max Planck Society

Catalytic systems based on bimetallic alloy nanoparticles (NPs) often exhibit significantly superior catalytic properties compared to their monometallic counterparts. The spatial atomic distribution in such bimetallic nanocatalysts plays a pivotal role in their efficiency and stability. Employing near-ambient pressure (NAP-XPS) and ultrahigh vacuum X-ray photoelectron spectroscopy (XPS) together with atomic force microscopy (AFM), surface segregation, restructuring, and sintering phenomena in size-controlled CuNi NPs supported on SiO_2/Si substrates were systematically investigated as a function of temperature, chemical state, and reactive gas environment [1]. The depth profile of the elemental composition of the particles was determined under operando CO_2 hydrogenation conditions by varying the X-ray photon energy. The morphological changes induced by adding CO to the reaction mixture were investigated. Our study showed that the initial chemical state of the NPs and the adsorbate-induced effects sensitively affect restructuring in CuNi nanocatalysts, suggesting that their surface atomic composition and thus their catalytic properties can be tuned by appropriate plasma and annealing treatments.

[1] Pielsticker et al., J. Phys. Chem. B, Just Accepted Manuscript (2017), DOI: 10.1021/acs.jpcb.7b06984.

O 7.7 Mon 12:00 MA 141

Preparation and catalytic properties of chitosan supporting sliver-based composite — •Yuhan Wu[1], Yang Xu[1], Chenglin Zhang[1], Zhiyong Liu[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany — [2]School of Chemistry & Chemical Engineering, Shihezi University, 832003 Shihezi, P. R. China

In this study, we reported two novel silver-based composite, Ag nanoparticles/N-doped carbon composite (Ag/NC) and Ag/AgCl loaded N-doped carbon composite photocatalyst (Ag/AgCl/NC). At first, Ag/NC was fabricated by a facile and green one-step hydrothermal treatment, during this progress the environmentally benign and renewable natural chitosan was used as not only reducer and stabilizer, but also as a nitrogen source and carbon source. Secondly, Ag/AgCl/NC composite photocatalyst was synthesized via in situ oxidation reaction by adding FeCl3. The Ag/NC and Ag/AgCl/NC were characterized using X-ray diffraction, transmission electronic microscopy, energy dispersive X-ray spectra, UV-visible diffused reflectance spectra, X-ray photoelectron spectroscopy and nitrogen adsorption-desorption measurements, respectively. The obtained two kinds of composite exhibited superior catalytic activity and stability for the degradation of organic contaminants.

O 7.8 Mon 12:15 MA 141

Decreasing the Pressure Gap: High-Pressure Low-Energy Electron Microscopy — •Benjamin Borkenhagen[1], Thorsten Franz[2], Bernhard von Boehn[3], Ronald Imbihl[3], Czeslaw Koziol[2], Winfried Daum[1], and Gerhard Lilienkamp[1] — [1]IEPT, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld — [2]ELMITEC GmbH, Albrecht-von-Grodeck-Str. 3, 38678 Clausthal-Zellerfeld — [3]PCI, Leibniz Universität Hannover, Callinstraße 3A, 30167 Hannover

Low-energy electron microscopy (LEEM) is a powerful tool for real-time studies on single crystal and polycrystalline surfaces, providing high surface sensitivity, chemical and structural contrast at lateral resolution as good as 2 nm. However, it is limited to vacuum environments with pressures below 10^{-5} mbar. High-pressure LEEM extends the accessible pressure range to 0.1 mbar and beyond, enabling microscopic in situ investigations of dynamic processes within a broad range of reaction conditions. We introduce high-pressure LEEM and present results from first high pressure experiments, including surface modification by oxidation and a catalytic surface reaction.

O 7.9 Mon 12:30 MA 141

Scanning tunneling microscopy study of the structure and interaction between carbon monoxide and hydrogen on the Ru(0001) surface — •Barbara A J Lechner[1,2], Xiaofeng Feng[1], Peter J Feibelman[3], Jorge I Cerdá[4], and Miquel Salmeron[1] — [1]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [2]Department of Chemistry & Catalysis Research Center, Technical University of Munich, Germany — [3]Sandia National Laboratories, Albuquerque, NM, USA — [4]Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC, Cantoblanco, 28049 Madrid, Spain

As the earth's crude oil supply dwindles, the Fischer-Tropsch process to create hydrocarbon fuels from two abundant resources, carbon monoxide and hydrogen, gains in significance. Here, we use scanning tunneling microscopy (STM) to investigate the spatial arrangement of CO and H coadsorbed on a model catalyst surface, Ru(0001). We find that at cryogenic temperatures, CO forms small triangular islands of up to 21 molecules with hydrogen segregated outside of the islands. Furthermore, whereas for small island sizes (3-6 CO molecules) the molecules adsorb at hcp sites, a registry shift toward top sites occurs for larger islands (10-21 CO molecules). To characterize the CO structures better and to help interpret the data, we carried out density functional theory (DFT) calculations of the structure and simulations of the STM images, which reveal a delicate interplay between the repulsions of the different species.

O 7.10 Mon 12:45 MA 141

High-pressure STM study of the low-temperature Fischer Tropsch synthesis on Co(0001) — •Bernhard Böller, Katharina Durner, and Joost Wintterlin — Ludwig-Maximilians-Universität, Munich

We report an operando high-pressure STM study of a Co(0001) single crystal model catalyst, performed under several 100 mbar of syngas (2 : 1 mixtures of H2 and CO) at 493 K. Under these conditions, ethane and propane can be detected as products, in addition to methane, which is in contrast to previous experiments performed at 10 mbar and at higher H2-to-CO ratios that only gave methane. The experiments thus represent a critical step toward the actual Fischer Tropsch synthesis of higher hydrocarbons. Massive problems had to be solved with respect to gas cleanliness, in particular from sulfur compounds and Ni(CO)4 that decomposed on the sample surface to give sulfur and nickel. These contaminants led to strong effects on the surface that can misleadingly indicate morphology changes induced by the reaction conditions. However, after extensive experimental measures the surface could be kept free from S and Ni on the timescale of hours. Also the amounts of surface carbon and oxygen, as measured by ex situ XPS, were low. Under these conditions, atomically resolved STM data showed no significant changes of the surface morphology, except for an enhanced mobility of steps, in contradiction to established models of the low-temperature Fischer Tropsch synthesis.

O 8: Solid-liquid interfaces: Structure, Spectroscopy I

Time: Monday 10:30–13:00 Location: MA 144

O 8.1 Mon 10:30 MA 144

Structural changes of water islands due to kosmotropes vs. chaotropes imaged in real space — •Irene Weber and Karina Morgenstern — Chair of Physical Chemistry I, Ruhr-Universität Bochum, Germany

Solvation effects of ions near the liquid-solid interface are of tremendous importance for the understanding of electrochemical processes, i.e. in electrocatalysis or in corrosion. Although studying these solvation effects has a long tradition, the understanding of the microscopic influence of alkali metal ions onto water structure and dynamics near metal surfaces on the atomic scale is still at its infancy. In our study, crystalline water is used to mimic ordered water close to an electrode and lithium or cesium ions to represent circular cations. Lithium with its high charge density is a kosmotrope and cesium with its low charge density a chaotrope. Already, the adsorption of lithium and cesium ions on the Au(111) surface differs at around 215 K. Both ions change the water structure. The lithium ions change the distribution of water islands on Au(111) as compared to water islands on pristine Au(111) and alter their structure. The cesium ions reduce the height of the islands and change the structure of water islands in a different way. Depending on the water-to-ion-ratio, the subtle balance of interactions between water, ions and the substrate is changed. In this contribution, we will present our variable-temperature Scanning Tunneling Microscopy (STM) studies of these differences induced by lithium and cesium ion co-adsorption on crystalline ice structures on Au(111).

O 8.2 Mon 10:45 MA 144

In-situ and operando near sulfur K-edge X-ray absorption spectrometry of Li-S battery coin cells — •Claudia Zech[1], Olga Grätz[2], Svetlozar Ivanov[3], Daniel Grötzsch[4], Philipp Hönicke[1], Yves Kayser[1], Manfred Stamm[2] und Burkhard Beckhoff[1] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Leibniz-Institut für Polymerforschung, Dresden, Germany — [3]Technische Universität, Ilmenau, Germany — [4]Technische Universität, Berlin, Germany

Lithium Sulfur (Li-S) batteries are promising candidates for improved batteries offering up to 5 times higher capacity than conventional lithium ion batteries. For a better understanding of battery degradation processes in-situ and in-operando characterization techniques are required. By means of in-operando near sulfur K-edge X-ray absorption spectrometry recorded during galvanostatic cycling with potential limitation (GCPL) measurements we could determine the different sulfur species for 8 cycles of a Li-S battery with DOL/DME (1:1 wt.%) 1 Mol TFSI electrolyte. In particular, the formation of polysulfides could be revealed. We used CR-2032 coin cell formed Li-S batteries modified with thin windows enabling the transmission of excitation and fluorescence radiation. Traceable X-ray spectrometric measurements were performed using radiometrically calibrated instrumentation in the PTB laboratory at BESSY II synchrotron radiation facility. While for the first cycles the polysulfides convert almost entirely we see for further cycles a permanent appearance.

O 8.3 Mon 11:00 MA 144

Structure of electrochemical electrode-electrolyte interfaces — •Florian Gossenberger and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

In electrochemistry, the atomistic structure at the solid-liquid interface has a strong influence on electrocatalytic reactions. Therefore it is of fundamental importance to understand surface properties like adsorbate structures at particular thermodynamic conditions e.g. pH, electrolyte-concentration and electrode potential first, before looking at any reaction at this interface. We adressed the structure of a Pt(111) electrode in a the presence of protons and halides in the electrolytes based on density functional theory calculations [1] using the concept of the computational hydrogen electrode (CHE). This represents an efficient method to combine total energy calculations from density functional theory with thermodynamic properties of electrochemistry. We have now extended these studies to analyze the co-adsorption of (bi)sulfate and hydrogen. We will discuss the important role of water molecules in stabilizing the resulting adsorbate structures.

[1] F. Gossenberger, T. Roman and A. Groß, Electrochim. Acta **216**, 152 (2016).

O 8.4 Mon 11:15 MA 144

Determination of the surface charge of the water-rutile (110) surface at low and high pH — •Shumei Sun, Mischa Bonn, and Ellen Backus — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We have used visible-infrared sum-frequency generation spectroscopy (SFG) to reveal the surface charge of the rutile (110) surface in contact with water of different pH. The surface is positively and negatively charged at pH3 and pH11, respectively, through protonation and deprotonation reactions. Phase-resolved SFG experiments show that under influence of the charged surface water molecules orient themselves with the hydrogen atoms towards (basic solution) or away from (acidic solution) the TiO2 surface. By combining a recently developed theoretical framework and salt concentration-dependent SFG measurements, we are able to near quantitatively evaluate the surface charge density at pH3 and pH11. The results reveal that the surface charge density of TiO2/pH11 is one order of magnitude smaller than that of TiO2/pH3. Moreover, by increasing the pH above 11, the surface charge is not increasing anymore.

O 8.5 Mon 11:30 MA 144

***Ab initio* description of semiconductor-water interfaces at finite electrode potential** — •Lei Yang[1], Fang Niu[1], Stefanie Tecklenburg[1], Simantini Nayak[1], Andreas Erbe[1], Francois Gygi[2], Giulia Galli[3], and Stefan Wippermann[1] — [1]MPI Eisenforschung — [2]UC Davis — [3]U 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. To develop robust strategies to interpret experiments and validate theory, we carried out attenuated total internal reflection (ATR-IR) spectroscopy measurements and *ab initio* molecular dynamics (AIMD) simulations of the vibrational properties of interfaces between liquid water and well-controlled prototypical semiconductor substrates. We show the Ge(100)/H_2O interface to feature a reversible potential-dependent surface phase transition from a hydrophilic to a hydrophobic surface. The Si(100)/H_2O interface is proposed as a model system for corrosion and oxidation processes. We performed *ab initio* time-resolved spectroscopy, providing a molecular-level explanation for the difference between the vibrational properties of the H_2O molecules on surfaces with different hydrophobicities on the basis of hydrogen bonding. Funding from DOE-BES Grant No. DE-SS0008939, Deutsche Forschungsgemeinschaft (RESOLV, EXC 1069) and BMBF NanoMatFutur Grant No. 13N12972 is gratefully acknowledged.

O 8.6 Mon 11:45 MA 144

GaP(100) in contact with water: Reflection anisotropy spectroscopy from first principles — •Matthias M. May and Michiel Sprik — Univeristy of Cambridge, Department of Chemistry

Surfaces of III-V semiconductors in contact with an electrolyte are not only relevant for applications such as solar water splitting, but also offer the opportunity to correlate experiments on well-defined surfaces with theory. Here, we study the P-rich surface of GaP(100), which shows an extraordinary stability against oxidation from gas-phase water. While its surface ordering is modified by exposure to water as evidenced by *in situ* reflection anisotropy spectroscopy (RAS), no traces of oxygen could be found by experiment.[1] Modelling the surface with density functional theory and deriving RAS, we find evidence for a water-induced hydrogen-rich surface phase. [2] We furthermore extend this work towards RAS in a bulk electrolyte by investigating the influence of finite electric fields and potentials [3] on the optical anisotropy in the Helmholtz layer.

[1] May et al, NJP 15:103003 (2013). [2] May and Sprik, arXiv:1710.08194. [3] Zhang and Sprik, PRB 94:245309 (2016).

O 8.7 Mon 12:00 MA 144

Molecular Dynamics of the Water-gold Interface including Metal Polarizability Effects in the Classical Force Field — •Victor G. Ruiz[1], Matej Kanduč[1], Won Kyu Kim[1], Rafael Roa[1], and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

Solid-liquid interfaces are of growing interest to basic science and technology. The water-gold interface has received much attention due to its applications in catalysis and biotechnology. The need of including biomolecular and ionic species in the aqueous environment within atomistic simulations necessitates the accurate inclusion of charge and fluctuations effects of the liquids [Small 12, 2395 (2016)]. The formed interfaces are complex due to the interplay of van der Waals (vdW) interactions, covalent bonds, and image-charge effects due to the highly polarizable surface. Using a classical Drude-oscillator model [JCP 119, 3025 (2003)], we present a force field for the gold-water interface which includes image-charge effects induced in the metal surface. Our parametrization is based on calculations of a single molecule/monolayer of water using vdW-corrected density-functional theory [PRL 108, 146103 (2012)] that includes the many-body collective response of the substrate electrons in the vdW interaction coefficients. We show that this methodology yields a consistent connection between the induced polarizability effects in the surface and the vdW interaction between water molecules and the surface when compared to available literature.

O 8.8 Mon 12:15 MA 144

Growth and dynamics of ultrathin ionic liquid layers on metal surfaces — •Matthias Lexow, Bettina Heller, Benjamin May, Radha G. Bhuin, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (IL) are ionic compounds with a relatively low melting point, often even below room temperature. In addition to numerous applications as a solvent or electrolyte, the extremely low vapour pressure of ILs also led to the development of completely new concepts for catalytically active systems. Thin layers of ILs on solid materials are applied e.g. in SCILL (Solid Catalyst with Ionic Liquid Layer) catalysis.

In this context, the structure and composition of the IL/solid interface is studied by our group combining in vacuo deposition of ultrathin IL films and angle-resolved X-ray photoelectron spectroscopy. The investigations show how the IL/solid interface forms and how to control the process by modifying the IL or substrate properties on the molecular scale.

Aiming to understand and predict the behaviour of applied catalyst systems, we discuss on the example of imidazolium based ionic liquids the role of the molecular structure in the mechanisms of initial film formation.

M.L., B.M, R.G.B and H.P.S. thank the European Research Council (ERC) for financial support of this research in the context of an Advanced Investigator Grant to H.P.S (No. 693398-ILID).

O 8.9 Mon 12:30 MA 144

Decisive Role of Nuclear Quantum Effects on Surface Mediated Water Dissociation at Finite Temperature — •Yair Litman[1], Davide Donadio[2], Michele Ceriotti[3], and Mariana Rossi[1] — [1]Fritz Haber Insitute of the Max Planck Society, Berlin, Germany — [2]University of California, Davis — [3]EPFL, Switzerland

Water molecules adsorbed on inorganic substrates play an important role in several technological applications. In the presence of light atoms in adsorbates, nuclear quantum effects (NQE) influence the structural stability and the dynamical properties of these systems. In this work [1], we explore NQE on the water dissociation of water wires on stepped Pt(221) surfaces. We note that there are several competing minima, calling for the inclusion of anharmonic effects in simulations at finite temperatures. We thus perform *ab initio* path integral molecular dynamics (PIMD) in order to calculate NQE contributions to free energies and their interplay with the electronic structure, making use of an acceleration technique that we propose, based on a spatially-localised ring-polymer contraction. We find that the dissociation process is dominated by ZPE, which can enhance the rate of dissociation by three orders of magnitude and that the inclusion of anharmonicities increase the nuclear quantum contribution to the dissociation free energy by 20 % compared to harmonic estimates. Interestingly, we report how the redistribution of electronic density caused by temperature and NQE can induce work function changes of up to 0.4 eV with respect to static estimates.

[1] Y. Litman *et. al.* JCP **148**, 102320 (2018).

O 8.10 Mon 12:45 MA 144

Surface plasmon resonance at electrified interfaces — •Ulmas E. Zhumaev and Katrin F. Domke — Max Planck Institute for Polymer Research, Mainz

Operating low-temperature fuel cells in the oscillatory regime is a promising approach to avoid the deactivation of platinum (Pt) catalyst by adsorbed carbon monoxide (CO). However, it remains an open question how to controllably activate the oscillatory regime. In the oscillatory regime, the Pt electrocatalyst undergoes spontaneous switching between the removal of adsorbed CO and the main reaction of the fuel cell. Such oscillations are accompanied by the formation of oscillatory CO concentration patterns on the Pt surface. Accessing these patterns with millisecond temporal and micrometer spatial resolutions using surface plasmon resonance (SPR) spectroscopy will help to gain insight into the oscillatory regime. To do so, the relationship between the SPR signal and the CO coverage under electrochemical (ec) conditions should be revealed. Our strategy is to define the contribution of different interfacial regions to the ecSPR signal by exploring well-known ec systems, e.g. Au(111) and Pt in $H_2SO_4/Cl^-/CO$, with SPR spectroscopy. Our first results on Au(111) and Pt/Au(111) in 0.1 M H_2SO_4 suggest a predominant contribution of specific adsorption to the SPR signal, whereas non-specific adsorption and diffusion processes seem to have almost no contribution. The contribution of the surface charge seems to be rather complex and we present experimental approaches towards its understanding.

O 9: Focus Session: Frontiers in Reducible Oxide Surface Science I

Time: Monday 10:30–13:00 Location: HFT-FT 131

Invited Talk O 9.1 Mon 10:30 HFT-FT 131
CeO_2(111) defect structure, oxygen migration and polaron hopping: A theoretical perspective — •M. Veronica Ganduglia-Pirovano[1], Gustavo E. Murgida[2], Valeria Ferrari[2], Ana Maria Llois[2], Dawei Zhang[3], Zhong-Kang Han[3,4], and Yi Gao[3,4] — [1]ICP-CSIC, Madrid — [2]CAC-CNEA, CONICET, Bs. As. — [3]SINAP-CAS, Shanghai — [4]UCAS, Beijing

Deep understanding of the defect structure of ceria(CeO_2) surfaces is essential to tailor their functionality in applications. For the CeO_2(111) surface, whether surface oxygen vacancies attract or repel, and whether oxygen migration and polaron (Ce^{3+}) hopping are entangled, are heavily debated. Also, a number of surface reconstructions have been observed upon reduction, but their structures have remained elusive. Here, supported by density-functional theory-based modeling, statistical thermodynamics, Monte Carlo and molecular dynamic simulations, and experimental results, we elucidate: (*i*) the subsurface preference at low vacancy concentration and temperature [1,2], (*ii*) the formation of surface vacancy clusters with increased degree of reduction and temperature [2], (*iii*) the nature of the observed $(\sqrt{7}\times\sqrt{7})R19.1^\circ$, $(\sqrt{7}\times 3)R19.1^\circ$, $(\sqrt{3}\times\sqrt{3})$, (3×3), and (4×4) reconstructions [3], as well as (*iv*) the role of Ce^{3+} ions in oxygen vacancy migration [4].
[1] G. E. Murgida, M. V. Ganduglia-Pirovano, Phys. Rev. Lett. 110. 246101 (2013).
[2] Z.-K. Han *et al.*, submitted to Phys. Rev. Materials (2017).
[3] R. Olbrich *et al.* J. Phys. Chem. C, 121, 6844 (2017).
[4] D. Zhang *et al.* in preparation.

Invited Talk O 9.2 Mon 11:00 HFT-FT 131
Interactions at the interface between cerium oxide and metals — •Paola Luches — Istituto Nanoscienze, CNR, Modena, Italy

The interaction between cerium oxide and metals leads to important modifications of the properties of the two materials, which are exploited in many different applications. Surface science studies have largely contributed to the understanding of these interfacial effects at the atomic scale.

I will show the results of our studies of model systems in the form of cerium oxide ultrathin films, focusing on the interplay with Pt in the form of a single crystal (111) oriented substrate. I will discuss the effects of metal proximity in terms of interface charge transfer [1] and atomic exchange. The influence of the metal substrate on the oxide structure and reducibility will also be described [2,3]. In addition, I will present the case in which the metal is in the form of nanoparticles supported on the cerium oxide film surface, discussing the case of Ag in detail [4,5].

I will finally show some promising research directions towards the exploitation of the interaction between cerium oxide and plasmonic metals, aimed at inducing additional functionalities to the composite system.
[1] P. Luches, et al. Adv. Mater. Interfaces 2, 1500375 (2015).
[2] P. Luches, et al. Phys. Chem. Chem. Phys. 16, 18848 (2014).
[3] G. Gasperi, et al. Phys. Chem. Chem. Phys. 18, 20511 (2016).
[4] P. Luches, et al. J. Phys. Chem. C 116, 1122 (2012).
[5] F. Benedetti, et al. J. Phys. Chem. C 119, 6024 (2015).

Invited Talk O 9.3 Mon 11:30 HFT-FT 131
Unraveling surface chemistry Of C-H reforming reactions over Ni-CeOx(111) catalysts — •Sanjaya Senanayake — Brookhaven National Laboratory, Upton, NY 11973, USA

We have utilized a combination of model and powder catalysts composed of Ni and CeOx, employing in situ spectroscopies to elucidate the active state and mechanistic steps associated with C-H bond activation in the ethanol steam reforming (ESR) and Methane Dry Reforming (DRM) reactions. Our results reveal that surface layers of the catalyst substrate can be probed under dynamic reaction conditions using AP-XPS, revealing the surface as highly reduced and hydroxylated under reaction conditions while the small supported Ni nanoparticles are present as Ni0/NixC essential for the C-H conversion processes. In addition, in both reactions, a multifunctional, synergistic role is highlighted in which Ni, CeOx and the interface provide an ensemble effect in the active chemistry that activates C-H (Ethanol/Methane) and leads to H2. We correlate changes to the active phases leading to both C-C and C-H bond cleavage in ESR, and C-H and C-O in DRM but also for carbon accumulation or coking that are intrinsic properties of such reactions. The interface (Ni-ceria) facilitates the C-C bond breaking step while the pathways that lead to H2 production may occur from the recombination of OH and CHx species. Additionally, we discuss important insights into the stability and selectivity of the catalyst in the presence of co-reactants and the strategies that will help correlate improved catalyst design for selective bond breaking and forming processes.

O 9.4 Mon 12:00 HFT-FT 131
Progressive reduction from CeO_2 to Ce_2O_3 — •Reinhard Olbrich[1], Gustavo E. Murgida[2,3], Valeria Ferrari[2,3], Clemens Barth[4], Ana M. Llois[2,3], Michael Reichling[1], and M. Veronica Ganduglia-Pirovano[5] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany — [2]Departamento de Física de la Materia Condensada, GIyA, CAC-CNEA, 1650 San Martín, Buenos Aires, Argentina — [3]Consejo Nacional de Investigaciones Científicas y Técnicas - CONICET, C1033AAJ, Buenos Aires, Argentina — [4]Aix-Marseille University, CNRS, CINaM UMR 7325, 13288 Marseille, France — [5]Instituto de Catálisis y Petroleoquímica, Consejo Superior de Investigaciones Científicas- CSIC, 28049 Madrid, Spain

The progressive reduction from CeO_2 to Ce_2O_3 of a 180nm thick ceria film annealed in an ultra-high vacuum (UHV) environment at temperatures up to 1100 K is observed by direct imaging with a non-contact atomic force microscope (NC-AFM). By combining high-resolution NC-AFM imaging with spin-polarized DFT+U calculations, we identify four surface reconstructions namely $\sqrt{(7)} \times \sqrt{(7)}$R19.1° Ce_7O_{12}, $\sqrt{(7)} \times 3$R19.1° Ce_3O_5, $\sqrt{(3)} \times \sqrt{(3)}$R30° Ce_3O_5 and 1×1 Ce_2O_3. We combine DFT total energy calculations with statistical thermodynamics to explain the sequence of occurrence of the observed phases and their coexisting at evaluated temperatures. The $\sqrt{(7)} \times 3$ phase is the only phase that has an unexpected oblique rather than a hexagonal structure. This phase only exists as a thin reduced over layer and can not be prepared in the bulk.

O 9.5 Mon 12:15 HFT-FT 131
Covalent versus localized nature of 4f electrons in ceria — •Tomáš Duchoň[1], Marie Aulická[1], Eike F. Schwier[2], Hideaki Iwasawa[2], Chuanlin Zhao[3], Ye Xu[3], Kateřina Veltruská[1], Kenya Shimada[2], and Vladimír Matolín[1] — [1]Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, 18000 Prague 8, Czech Republic — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Hiroshima 839-0046, Japan — [3]Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana 70803, USA

4f electrons play an important role in the redox cycle of rare earth oxides. Here, we utilize isostructural transition between CeO2(111) and c-Ce2O3(111) to reveal the nature of 4f contribution in the valence band of cerium oxide. Separating intra- and interatomic photoemission processes via combined resonant angle-resolved photoemission spectroscopy and density functional theory investigation, we report on c-f hybridization and its modification through anion doping as a viable means of steering the surface chemistry of cerium oxide.

O 9.6 Mon 12:30 HFT-FT 131
Surface structure and reactivity of cerium oxide — •Chengwu

Yang, Alexei Nefedov, Yuemin Wang, and Christof Wöll — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany.

Ceria is becoming a ubiquitous constituent in catalytic systems for a variety of applications over the last forty years. The high catalytic activity is connected with its strong redox properties making ceria the ideal buffer system for oxygen in a catalytic process. The importance of this material has triggered numerous experimental and theoretical studies. The studies on bulk single crystal surfaces, however, are still scarce.

On a novel UHV-FTIRS we used carbon monoxide (CO) as probe molecule to detect the surface structure of ceria bulk single crystals and nanocrystals. Our results indicate that CO is capable of probing surface oxygen vacancies and distinguishing facet orientations. After the determination of ceria surface structure, the unexpected origin of photoreactivity of ceria has been investigated by monitoring the UV-induced decomposition of nitrous oxide (N2O) on well-defined single crystals of ceria. We demonstrate that ceria becomes photoactive only in the presence of surface O-vacancies with largely undercoordinated electron-rich Ce3+ cations. Additionally, we also provide direct spectroscopic evidence for the formation of active dioxygen species (superoxo and peroxo species) on the reduced ceria (110) and (100) surfaces upon oxygen (O2) adsorption. However, neither of these species was present on ceria (111).

O 9.7 Mon 12:45 HFT-FT 131

Spectroscopic evidence for the controlled formation of catalytically active Pt nanoparticles supported on ceria — •Junjun Wang, Alexei Nefedov, Christof Wöll, and Yuemin Wang — Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany

Ceria-supported Pt catalysts have received increased attention from both fundamental and technological perspectives due to their applications in several fields such as automotive exhaust cleaning and hydrocarbon reforming. It has been proposed that the catalytic activity and utilization efficiency of Pt can be significantly enhanced by decreasing the particle size to ultrafine clusters. In the present work, the surface structure and oxidation states of ceria-supported Pt nanoparticles under alternating reductive and oxidative conditions were monitored by ultrahigh vacuum IR spectroscopy using CO as a probe molecule. Our results provided direct spectroscopic evidence for the re-dispersion of Pt particles in ceria after oxidation at moderate temperatures. It was found that the subsequent reduction treatments at different temperatures lead to a controlled formation of ultrafine Pt particles. The combined IR and high-resolution XPS data allowed us to gain detailed insights into the strong Pt-ceria interaction and the dynamic behavior of Pt clusters under reductive and oxidative atmospheres.

O 10: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)

Exploring, understanding, and describing materials with strong electronic Coulomb correlations remain among the big challenges of modern condensed matter physics. Correlated materials are characterized by an extreme sensitivity to external probes such as pressure or temperature, and slight changes in composition, constraints during the growth process (e.g. by heterostructuring) or off-stoechiometries can significantly alter their properties. While the invited lectures will have a focus on correlated electron materials, the symposium will cover the general field of computational materials science and electronic-structure theory.

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Time: Monday 10:30–13:00 Location: HL 001

O 10.1 Mon 10:30 HL 001

How Derivative Discontinuities in the Energy Yield Interatomic Steps in the Exact Kohn-Sham Potential of Density-Functional Theory — •Eli Kraisler[1], Matthew J. P. Hodgson[1], Axel Schild[2], and Eberhard K.U. Gross[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [2]Laboratorium für Physikalische Chemie, ETH Zürich, Switzerland — [3]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Israel

Accurate density-functional calculations hinge on reliable approximations to the unknown exchange-correlation (xc) potential. The most popular approximations usually lack features of the exact xc potential that are important for an accurate prediction of the fundamental gap and the distribution of charge in complex systems. Two principal features in this regard are the spatially uniform shift in the potential, as the number of electrons infinitesimally surpasses an integer, and the spatial steps that form, e.g., between the atoms of stretched molecules. Although both aforementioned concepts are well-known, the exact relationship between them remained unclear. In this talk, we establish this relationship and introduce a new concept: the charge-transfer derivative discontinuity, Δ^{CT}. By numerically solving the many-electron Schrödinger equation, we extract the exact Kohn-Sham potential and directly observe its features, particularly the spatial interatomic steps. For the first time, spatial steps in the exact xc potential of a full configuration-interaction (FCI) calculation of a molecule are presented in three dimensions.

O 10.2 Mon 10:45 HL 001

Steps in the exact Kohn-Sham potential of ensemble density-functional theory for excited states and their relation to the derivative discontinuity — •Matthew J. P. Hodgson[1], Eli Kraisler[1], Michael T. Entwistle[2], Axel Schild[3], and Eberhard K. U. Gross[1,4] — [1]MPI für Mikrostrukturphysik, D-06120 Halle, Germany — [2]Dep. of Physics, Uni. of York, Heslington, YO10 5DD, UK — [3]Lab. für Physikalische Chemie, ETH Zürich, 8093, Switzerland — [4]Fritz Haber Center for Molecular Dynamics, The Hebrew University of Jerusalem, 91904, Israel

An accurate approximation to the exchange-correlation (xc) part of the Kohn-Sham (KS) potential is essential for any density-functional calculation. Understanding the behaviour of the exact xc potential and developing improved approximations to it are crucial. The focus of calculations within density functional theory is usually on the ground state. However, knowledge of how the system responds to an excitation is important. In this talk we present the exact KS potential of an ensemble of the ground state and the first excited state of a 1D diatomic molecule. For this system, upon excitation, a small amount of charge transfers from one atom to the other. In the corresponding exact ensemble xc potential we find two plateaus: one that forms around the nucleus of the acceptor atom, associated with the derivative discontinuity of that atom, and another that forms around the donor atom and corresponds to a new phenomenon which we term the 'charge-transfer derivative discontinuity'.

O 10.3 Mon 11:00 HL 001

Koopmans-compliant functionals: A reliable and efficient tool for the prediction of spectroscopic quantities — •Nicola Colonna[1], Ngoc Linh Nguyen[1], Andrea Ferretti[2], and Nicola Marzari[1] — [1]THEOS and MARVEL, EPFL, Lausanne, Switzerland — [2]Centro S3, CNR-Istituto Nanoscienze, Modena, Italy

Commonly used approximate density functionals produce total energies that do not exhibit the expected piecewise-linear behavior as a function of the particle number, leading to a discrepancy between total and partial electron removal/addition energies and poor predictive capabilities of ionization potentials. Koopmans-compliant functionals enforce a generalized criterion of piecewise linearity in the energy of any approximate density functional with respect to the partial removal/addition of an electron - i.e., with respect to charged excitations - from/to any orbital of the system. When used to purify approximate density functionals, Koopmans' corrections lead to orbital-density dependent functionals and potentials that are able to deliver accurate spectroscopic properties. As an example, ionization potentials of a large set of molecules (the GW100 test set), photoemission spectra of organic donors and acceptors and band gaps of 35 semiconductors and insulators are presented, showing very good agreement with experiment or higher-order theories. Being this a functional framework, the straightforward advantages are that forces and other derivatives are also readily accessible, that the computational costs are much reduced, and the numerical parameters are those typical of DFT calculations.

O 10.4 Mon 11:15 HL 001

Selfconsitent density embedding - a new class of functionals for DFT — •Uliana Mordovina[1], Teresa E. Reinhard[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

We propose a new technique to find functionals for density functional theory (DFT) in an ab-initio fashion. This technique origins in the recently developed density-matrix embedding theory (DMET) [1]. DMET is a quantum-in-quantum embedding method, which is based on finding a projection between the high-dimensional wave function of the full system and a lower-dimensional wavefunction living in the active space of the embedded system, which is then solved exactly. In the original DMET scope, the projection is improved via optimization of the reduced one-body density matrix. We replace this optimization by a density inversion, exploiting the one-to-one mapping between electronic density and Kohn-Sham potential.

The proposed density-embedding scheme serves as functional in DFT, which, unlike in usual DFT, can be systematically improved by increasing the size of the active space.

We show convergence toward exact results for 1D systems as well as results for 2D systems.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

O 10.5 Mon 11:30 HL 001

Pressure dependence of the effective screened Coulomb interactions in transition metal monoxides — •Swarup Kumar Panda[1], Hong Jiang[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, France — [2]College of Chemistry and Molecular Engineering, Peking University, China — [3]Collège de France, Paris, France

In transition metal compounds, the magnitudes of the effective Coulomb interaction parameters (Hubbard U) and their pressure dependence are of utmost importance in any realistic many-body simulations for describing their pressure driven insulator-metal transition. One of the powerful methods for calculating the Hubbard U from first principles is based on linear response theory within the constrained random-phase approximation (cRPA) [1], which provides the full U matrix including off-site elements and its frequency dependence. In this presentation, we apply this method (in its implementation into the Wien2k code [2]) to the transition metal monoxides (FeO, CoO, NiO, and CuO) [3]. Although the pressure induced changes in the bare Coulomb interactions are negligible, the effective screened U grows monotonically with increasing pressure for all of the above monoxides. Finally, I will argue that neither the pressure dependence nor the frequency dependence of U should be ignored in a reliable theoretical description of correlated oxides.

References: [1] Aryasetiawan et al., PRB 70, 195104 (2004) [2] Vaugier et al., PRB 86, 165105 (2012) [3] Panda et al., PRB 96, 045137 (2017)

O 10.6 Mon 11:45 HL 001

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

The self-interaction error (SIE) is a well-known problem in all semilocal density-functional approximations (DFAs), including the recently proposed "strongly constrained and appropriately normed" (SCAN) functional [1]. The so-called self-consistent Fermi-orbital SIC (FSIC) algorithm proposed by Pederson *et al.* [2] shows promising potential to eliminate the self-interaction error in semilocal approximations, which has been demonstrated for the local-spin-density approximation (LSDA) in a study of molecules.

We present an all-electron implementation of the self-consistent FSIC approach on the SCAN method [1]. Beside a systematic benchmark with respect to a selected molecular test set, we examine the performance of FSIC-SCAN in predicting the geometry of Pentacene, which is a well-documented challenge for standard semilocal DFAs [3]. Finally, we briefly discuss our ongoing work concerned with the implementation of the all-electron FSIC-SCAN approach for solids.

[1] J. Sun, A. Ruzsinszky, and J. P. Perdew, *Phys. Rev. Lett.* **115**, 036402 (2015).

[2] M. R. Pederson and T. Baruah, *Advances In Atomic, Molecular, and Optical Physics* **64**, 153 (2015).

[3] M. R. Pederson, T. Baruah, D. you Kao, and L. Basurto, *The Journal of Chemical Physics* **144**, 164117 (2016).

O 10.7 Mon 12:00 HL 001

Progress in Fermi-Löwdin orbital self-interaction correction to DFT — •Torsten Hahn[1], Sebastian Schwalbe[1], Simon Liebing[1], Mark Pederson[2], and Jens Kortus[1] — [1]TU Freiberg, Institute for Theoretical Physics, Germany — [2]Johns Hopkins University, Department of Chemistry, USA

The accuracy of density functional theory (DFT) calculations is limited by the so called self-interaction error [1]. The recently proposed Fermi-Löwdin orbital based method [2,3,4] for self-interaction correction (FLO-SIC) is a unitary invariant and size extensive approach to overcome this error. We present the current state of the method and discuss the performance of FLO-SIC DFT applied to atoms and molecules in combination with different exchange-correlation functionals. In addition, this method delivers a description of the chemical bonding as intuitive as Lewis theory that may bridge the gap between DFT and chemical intuition.

[1] J. P. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)

[2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)

[3] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)

[4] T. Hahn et. al., J. Chem. Phys., vol- 143, 224104 (2015)

O 10.8 Mon 12:15 HL 001

First-principles modeling of mixed-valence compounds from extended Hubbard-corrected functionals — •Matteo Cococcioni and Nicola Marzari — Theory and Simulations of Materials and MARVEL, EPFL, Lausanne, Switzerland

Modeling the electronic properties of mixed valence compounds is central to developing many materials of technological relevance. Unfortunately, most approximate implementations of density functional theory (DFT) fail in capturing the localization of valence electrons on low dispersion states (e.g., of d or f kind) and mis-represent many properties of these systems. Quantitatively predictive first-principles calculations thus require, for these systems, the use of corrective functionals able to improve the description of electronic localization. Using the results of a recent study on materials for cathodes of Li-ion batteries this work shows how an extended Hubbard correction to DFT functionals, including on-site (U) and inter-site (V) interactions (named DFT+U+V) improves considerably on simpler approximations for electronic, magnetic and structural properties and correctly describes localized states even in presence of significant inter-site hybridization. The work also demonstrates that evaluating the effective interaction parameters (U and V) consistently with the electronic and crystal structures, and treating them as material-specific quantities, improves the prediction of thermodynamic quantities and of average voltages. Finally, a novel method to compute these interactions from density-functional perturbation theory is shown to guarantee unprecedented efficiency, accuracy and convergence control.

O 10.9 Mon 12:30 HL 001

A Kohn-Sham type construction on a lattice with the exact kinetic energy density — •Iris Theophilou[1], Michael Ruggenthaler[1], Florian Buchholz[1], Florian Eich[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In this presentation we explore a possible formulation of ground state Density Functional Theory by introducing the kinetic energy density as basic quantity in addition to the density. We presently restrict this formulation to the lattice case, and show that for a few site Hubbard interacting model it is numerically feasible to find an equivalent non-interacting system that yields the same density and kinetic energy density. By finding such a non-interacting system we mean here finding the local/on site potential and the non-local site dependent hopping that will give the target density and kinetic energy density. Our hope is that by including the kinetic energy density we will facilitate the functional construction and also put into grounds already existing approximations based on this quantity.

O 10.10 Mon 12:45 HL 001

Small-Polaron Formation in Polymorphs of Ga_2O_3 and TiO_2 — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin 14195, Germany

Transparent oxides are key materials for new devices in photovoltaics and electronics. One important factor influencing the behavior of charge carriers in these materials is the interaction with polar phonon modes. We focus on materials with strong electron-phonon coupling, where small polarons are formed. Although, density-functional theory (DFT) is often used for calculating polaron properties, there are two challenges: Sensitivity of the calculated properties to the errors in exchange-correlation treatment, and finite-size effects in supercell calculations. We have developed an approach [1] to address these issues. The polaron properties are obtained using a modified neutral potential-energy surface from DFT [2]. Based on Pekar′s model [3], we correct for the proper elastic long-range behavior of the polaron in a supercell. With this approach, the influence of the crystal structure on the polaron properties is investigated for rutile and anatase TiO_2, and for the monoclinic β– and orthorhombic ε–Ga_2O_3. We find that in rutile TiO_2 only small electron polarons are stable, while only small hole polarons are found in anatase. On the contrary, small hole polarons exist in both Ga_2O_3 polymorphs but have significantly different binding energies.
[1] S. Kokott, arXiv:1710.03722 (2017)
[2] B. Sadigh et al., Phys. Rev. B **92**, 75202 (2015)
[3] S. I. Pekar, Zh. Eksp. Teor. Fiz. **16** 335 (1946)

O 11: Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures I

This focus session aims at covering recent progress in both the formation and understanding of complex molecular architectures on surfaces. The bottom-up fabrication of surface-supported molecular architectures is either based on molecular self-assembly utilizing non-covalent intermolecular interactions or covalent on-surface synthesis. The intention is to provide a platform for discussing important aspects of molecular ensembles in contact with metallic, semi-conducting, and insulating substrates. In the focus are recent advances in theory as well as experiments dealing with single molecule chemistry, the understanding and controlled growth of complex molecular self assemblies and on surface synthesis of covalent structures.

Organizers: Sabine Maier, FAU Erlangen-Nürnberg; Meike Stöhr, University of Groningen

Time: Monday 15:00–18:15 Location: MA 004

Invited Talk O 11.1 Mon 15:00 MA 004

Elementary phenomena in hybrid graphene nanoribbons on surfaces — •Nacho Pascual — CIC nanoGUNE, San Sebastian (Basque Country)

Graphene nanoribbons (GNR) are cornerstone materials for functional devices, but their properties strongly depend on atomic-scale details of their structure. On-surface synthesis strategies can produce them on a metal surface and control their shape with atomic precision by clever selection of organic precursors [1]. The physics of these carbon structures is full of elementary phenomenology that can be accessed with great detail combining high-resolution STM imaging with local spectroscopy. These ribbons behave as one-dimensional semiconductors with band structure that depends on their width [2] and growth direction [3], and can be tuned by doping them with chemical groups at their edge [4]. The functional character of the ribbons is enhanced when two or more precursors are mixed into hybrid ribbons, resulting in, for example, quantum electron boxes [5] embedded in the carbon backbone. To date, magnetism has been elusive in GNR structures. By incorporating magnetic species in the synthesis steps we created hybrid porphyrin-GNR molecular devices. We show that the molecular spin survives in the ribbon by using spin-excitation inelastic spectroscopy. [1] K. Cai et al., Nature 466, 470 (2010) [2] N. Merino et al., ACS nano 11, 11661 (2017) [3] D.G. de Oteyza et al., ACS Nano 10, 9000 (2016) [4] E.Carbonell et al., ACS Nano 11, 7355 (2017) [5] E. Carbonell et al., Nano Letters 17, 50 (2017)

O 11.2 Mon 15:30 MA 004

Hierarchical On-Surface Synthesis of Deterministic Graphene Nanoribbon Heterojunctions — •Christopher Bronner[1], Rebecca A. Durr[2], Daniel J. Rizzo[1], Yea-Lee Lee[1,3], Tomas Marangoni[2], Alin Miksi Kalayjian[2], Henry Rodriguez[1], William Zhao[1], Steven G. Louie[1,4], Felix R. Fischer[2,4,5], and Michael F. Crommie[1,4,5] — [1]Dept. of Physics, University of California, Berkeley, United States — [2]Dept. of Chemistry, University of California, Berkeley, United States — [3]Dept. of Physics, Pohang University of Science and Technology, Korea — [4]Materials Sciences Division, Lawrence Berkeley National Laboratory, United States — [5]Kavli ENSI, Berkeley, United States

Heterojunctions of two dissimilar bottom-up fabricated graphene nanoribbons (GNRs) provide a platform for new functional devices on the molecular scale. Their on-surface synthesis via copolymerization of two different Br-substituted precursors has been previously reported, but unselective copolymerization results in random sequences of the two constituting GNRs. We demonstrate on-surface synthesis of non-random GNR heterojunctions employing a hierarchical growth strategy. Using both I and Br-substituted precursors with different halogen bond strengths as well as a bifunctional linker molecule allows us to grow the two different segments sequentially. The resulting block-copolymers translate into deterministic GNR heterostructures of two chevron-GNRs joined in only one heterojunction, suitable for device integration.

O 11.3 Mon 15:45 MA 004

Edge states in chiral-shaped graphene nanoribbons. — •Néstor Merino-Díez[1,2], Jingcheng Li[2,3], Aran García-Lekue[1,4], Sofía Sanz[1], Thomas Frederiksen[1], Diego Peña[5], Dimas G. de Oteyza[1,4], and Jose Ignacio Pascual[2,4] — [1]Donostia International Physics Center (DIPC) , 20018 San Sebastián (Spain) — [2]CIC Nanogune, 20018 San Sebastián (Spain) — [3]Centro de Física de Materiales (CFM), 20018 San Sebastián, (Spain) — [4]Ikerbasque, 48013 Bilbao (Spain) — [5]Centro de Investigación Química Biolóxica e Materiais Meloculares (CIQUS), 15782 Santiago de Compostela (Spain)

Understanding the configuration of electrons in graphene nanoribbons (GNRs), and the physical phenomena beneath, is still a challenging quest. Among all the GNRs studied to date, chiral-shaped GNRs (i.e. with periodically alternating armchair and zigzag-like segments) represent the most scarcely explored ones.

Recently we reported the growth of narrow chiral GNRs (alternating 3 zigzag-1 armchair segments) by depositing pre-designed molecular precursors on different coinage metallic surfaces [D.G. de Oteyza et al., ACSnano 10, 9000-9008 (2016)]. This ribbon presents a small semiconducting gap of 670mV [N. Merino-Díez et al., arXiv: 1710.05813]. Here we present the on-surface synthesis of wider chiral GNRs by using molecular precursors with additional anthracene units. Using scanning tunnelling spectroscopy we demonstrate that the width strongly determines the formation and shape of electronic edges states.

O 11.4 Mon 16:00 MA 004

Topological modifications in graphene nanostructures — •Shantanu Mishra, Carlo A. Pignedoli, Pascal Ruffieux, and Roman Fasel — Empa - Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

Graphene is the first two-dimensional crystal discovered in nature. The interesting properties of graphene arise from the sp2-network of carbon atoms and a perfect arrangement of hexagonal rings. Like any other crystal, presence of defects disrupting the pristine topology should significantly impact the physical properties of graphene. Introduction of defects thus provides a platform to tailor intrinsic properties of graphene and mandates a rational approach to achieve atomic-scale control over construction and implementation of defects for device applications. Regarding this, on-surface Ullmann reaction has become an indispensable synthetic tool to achieve atomically precise synthesis of nanostructures.

Utilizing this synthetic procedure, we fabricate two novel graphene nanostructures. The first is a non-alternant polyaromatic hydrocarbon demonstrating the first rational synthesis of the inverse Stone-Thrower-Wales defect in graphene. The second structure constitutes an organic polymer with precise substitution of specific carbon atoms with nitrogen atoms, that presents a model case for doping of graphene nanostructures with possible introduction of magnetism. Using a combined scanning tunneling microscopy and density functional theory based study, we investigate the novel properties that these altered bond or atomic topologies impart to nanographenes.

O 11.5 Mon 16:15 MA 004

Electronic band structure of poly (meta-phenylene) zigzag chains — •Ignacio Piquero-Zulaica[1], Aran García-Lekue[2,3], Claudio K. Krug[4], J. Enrique Ortega[1,2,5], J. Michael Gottfried[4], and Jorge Lobo-Checa[6,7] — [1]Centro de Física de Materiales CSIC/UPV-EHU, San Sebastian, Spain — [2]Donostia International Physics Center, San Sebastian, Spain — [3]Ikerbasque, Basque Foundation for Science, Bilbao, Spain — [4]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [5]Universidad del País Vasco, Dpto. Física Aplicada I, San Sebastian, Spain — [6]Instituto de Ciencia de Materiales de Aragón (ICMA), CSIC-Universidad de Zaragoza, Spain — [7]Departamento de Física de la Materia Condensada, Universidad de Zaragoza, Spain

Carbon based low-dimensional nanostructures such as on-surface synthesized Graphene nanoribbons (GNRs) and oligophenylene chains provide a vast playground for developing organic semiconductors with specific electronic properties. For instance, recent ARPES band structure studies on macroscopically aligned poly (para-phenylene) (PPP) and armchair-GNRs unraveled highly dispersive electronic bands with a large HOMO-LUMO gap. Analogously, we generate atomically precise and aligned on-surface synthesized poly (meta-phenylene) (PMP) zigzag chains on a curved Ag(111) surface. With the use of ARPES, we unravel its band structure for the first time and find weakly dispersive bands with considerably increased HOMO-LUMO gap. These results, supported with DFT calculations, suggest a strong tunability of the polymer's electronic properties that we can correlate to its topology.

15 min. break

O 11.6 Mon 16:45 MA 004

DFT study of super-atom states in graphene nanoribbons — •Bernhard Kretz[1] and Aran Garcia-Lekue[1,2] — [1]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, E-48013 Bilbao, Spain

In the two dimensional plane of graphene image states exist in the vacuum region above and below the graphene layer.[1] Such states do not follow the atomic lattice modulation and behave as nearly-free electrons (NFE). When graphene is rolled into nanotubes or fullerenes, these states overlap giving rise to the emergence of 1D NFE bands or 0D Super-Atom Molecular Orbitals (SAMOs).[2,3] In this work, we analyze a similar scenario in a reduced dimension, when the extended image states are related to the 1D edge of graphene. Using density functional theory (DFT), we investigate the emergence of 1D-NFE states in graphene nanoribbons, and we propose a way to confine them by modulating the width of the ribbons periodically, thus effectively creating 0D-SAMOs. Interestingly, the existence of a related SAMO state in the central empty region of a carbon-based macromolecule has been recently reported.[4]

[1] V. M. Silkin, et al., Phys. Rev. B, 80, 121408(R), 2009
[2] S. Hu et al., Nano Lett. 10, 4830 (2010)
[3] M. Feng et al., Science, 320, 359-362, 2008
[4] J. Heuille et al. (submitted)

O 11.7 Mon 17:00 MA 004

Precise mono-selective aromatic C-H activation by chemisorption of meta-aryne on a metal surface — •Qitang Fan[1], Simon Werner[1], Jalmar Tschakert[2], Daniel Ebeling[2], André Schirmeisen[2], Wolfgang Hieringer[3], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Institute of Applied Physics (IAP), Justus Liebig University Gießen, Germany — [3]Lehrstuhl für Theoretische Chemie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Aromatic C-H activation has attracted much attention due to their wide range of applications in the synthesis of aryl-containing chemicals. The major challenge lies in the minimization of the activation barrier and maximization of the regioselectivity. Here, we report the Cu(111) surface-catalyzed highly-selective activation of the C-H bond between two meta-substituted C-Br groups anchored on a phenyl ring. Two prototype molecules, i.e., 4',6'-dibromo-meta-terphenyl and 3',5'-dibromo-ortho-terphenyl have been employed to perform reactions on Cu(111). The chemical structures of the resulted products have been clarified by the combination of scanning tunneling microscopy and noncontact atomic force microscopy. Both of them demonstrate a remarkable weakening of the C-H bond between the two C-Br groups. Density function theory reveals that this efficient C-H activation stems from the extraordinary chemisorption of the meta-aryne, which leads to the close proximity of the targeted C-H bond to the Cu(111) surface and the out-of-plane deformation of the phenyl ring. These findings pave the way for new types of C-H activation approaches.

O 11.8 Mon 17:15 MA 004

A novel surface-catalytic reaction studied by scanning probe microscopy — •Lacheng Liu[1,2], Hong-Ying Gao[1,2], Henning Klaasen[3], Alexander Timmer[1,2], Harry Mönig[1,2], Armido Studer[3], and Harald Fuchs[1,2] — [1]Center for Nanotechnology, Heisenbergstraße 11, 48149 Münster, Germany — [2]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [3]Organisch-Chemisches Institut and Center for Mutiscale Theory and Simulation, Westfälische Wilhelms-Universität Münster, Corrensstraße 40, 48149 Münster, Germany

On-surface synthesis is a promising surface-assisted approach to form novel functional nanostructures via covalent interaction between organic molecules. In this work, we report a novel surface-catalytic reaction on Au(111), Cu(111) and Ag(111) surfaces with the same organic molecule as precursors. The scanning tunneling microscopy (STM) imaging study shows that two different 1D covalent polymers will be formed on metal surfaces via two steps of thermal annealing, respectively. The polymerization occurs at lower thermal annealing temperature on Cu(111) than that of on Au(111) and Ag(111). To understand the pass way of the reaction on metal surfaces, non-contact atomic force microscopy (nc-AFM) and X-ray photoelectron spectroscopy (XPS) measurements were performed combined with DFT calculation. The novel reaction provides a promising way to synthesis 1D polymers on metal surfaces.

O 11.9 Mon 17:30 MA 004

On-surface synthesis of indenofluorene polymers using methyl groups to form 5-membered rings — •Marco Di Giovannantonio[1], José I. Urgel[1], Aliaksandr Yakutovich[1], Jan Wilhelm[2], Uliana Beser[3], Akimitsu Narita[3], Carlo A. Pignedoli[1], Pascal Ruffieux[1], Klaus Müllen[3], and Roman Fasel[1,4] — [1]Empa - Swiss Federal Laboratories for Materials Science and Technology, nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland — [2]University of Zurich, Department of Chemistry, 8057 Zurich, Switzerland — [3]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [4]Department of Chemistry and Biochemistry, University of Bern, 3012 Bern, Switzerland

On-surface synthesis has opened pathways to molecular nanostructures that have been inaccessible so far. Here, we show the surface-assisted aryl-aryl coupling of brominated precursor molecules, followed by the cyclization of methyl groups on a poly(para-phenylene) backbone to form 5-membered rings, and to realize a fully conjugated chain composed of indenofluorene units. Indenofluorenes are appealing molecules consisting of an array of fused 6-5-6-5-6-membered rings with 20 π-electrons, which have received increasing attention for their formal anti-aromaticity, open-shell biradical character, and narrow HOMO-LUMO gap. The structure and electronic properties of the obtained indenofluorene polymers have been characterized by STM, nc-AFM, and STS, which are supported by theoretical calculations. The reported synthetic protocol can potentially be extended to other novel molecular nanostructures to fine tune their electronic properties.

O 11.10 Mon 17:45 MA 004

On-surface formation of cumulene by dehalogenative homocoupling — Bay Tran[1], Qiang Sun[2], •Mihaela Enache[1], Liangliang Cai[2], Honghong Ma[2], Xin Yu[2], Chunxue Yuan[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Groningen, Netherlands — [2]Interdisciplinary Materials Research Center, Tongji University, Shanghai, China

Recently, on-surface synthesis based on the use of covalent linking has offered an excellent platform to construct novel 1D and 2D carbon-based materials. In particular, the thermally induced dehalogenation of pre-defined C-X groups (X = halogen) provides an efficient route to produce radicals for subsequent C-C couplings on the surface [1]. Until now, all employed halide precursors had only one halogen attached to a carbon atom. It is thus of interest to study the effect of attaching more than one halogen atom to a carbon atom with the aim of producing multiple unpaired electrons.

Herein, by introducing an alkenyl gem-dibromide, cumulene products were fabricated on an Au(111) surface by dehalogenative homocoupling reactions [2]. The reaction products and pathways were unambiguously characterized by the combination of high-resolution scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) measurements together with density functional theory (DFT) calculations.

[1] B.V. Tran et al., Nanoscale, DOI : 10.1039/C7NR06187K

[2]Q. Sun et al., Angew. Chem. Int. Ed. 56, 12165-12169 (2017).

O 11.11 Mon 18:00 MA 004

Self-assembly and on-surface reaction of bromo-substituted decacyclene on Ag(111) — •Shadi Sorayya[1], Sachin Menon[1], Jörg Tomada[2], Konstantin Amsharov[2], and Sabine Maier[1] — [1]Department of Physics, FAU Erlangen-Nürnberg — [2]Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg

Controlling and understanding the self-assembly of chiral molecular building blocks on surfaces is essential for chiral separation and recognition. Here, we report on the self-assembly and on-surface reaction of chiral bromo-substituted decacyclene molecules adsorbed on Ag(111) using high-resolution scanning tunneling microscopy at low temperatures. The steric repulsion between adjacent hydrogen atoms at the peripheral naphthalene units of the decacyclene derivative leads to a twist in the molecular scaffold, and hence several chiral conformers are found upon adsorption on the surface. We observe compact and porous organo-metallic networks upon annealing because of the complex interplay between intermolecular forces and chirality of the constituent molecules. The structural properties of the networks and the chirality will be discussed in detail. Interestingly, we see a transition from homochiral to heterochiral networks upon annealing.

O 12: Ultrafast Electron and spin dynamics at interfaces II

Time: Monday 15:00–18:15 Location: MA 005

O 12.1 Mon 15:00 MA 005

Excited states mapping of a transition metal dichalcogenide semiconductor — •Michele Puppin[1,2], Chris Nicholson[1], Adriel Domínguez García[3], Hannes Huebener[3], Angel Rubio[3], Laurenz Rettig[1], Martin Wolf[1], and Ernstorfer Ralph[1] — [1]Fritz-Haber Institut, Berlin Germany — [2]École polytechnique fédérale de Lausanne, Lausanne Switzerland — [3]Max Planck Institut for the dynamics of matter, Hamburg, Germany

Time-resolved photoemission combined with scanning of the emission angle can extend established band-structure mapping to excited states which are only occupied out-of-equilibrium. The full potential of time- and angle-resolved photoemission spectroscopy (trARPES) is reached by performing the experiment at high repetition rates of hundreds of kHz, limiting space charge effects and data acquisition time. Extreme ultraviolet (XUV) photon energies grant access to the whole Brillouin zone: by performing high-harmonic generation at 0.5 MHz with a novel laser light source, we demonstrate trARPES with a photon energy of 21 eV, $\approx$100 meV resolution and sub-50 fs time resolution. A 3.1 eV pump pulse populates the conduction band of the layered transition metal dichalcogenide WSe2 followed by relaxation toward the band minimum within 1 picosecond. About 100 fs after excitation, most of the normally unoccupied conduction band states are populated due to scattering of the photo-excited carriers, allowing excited state band mapping throughout the whole Brillouin zone.

O 12.2 Mon 15:15 MA 005

Ultrafast dynamics in bilayer MoS_2 — •Klara Volckaert[1], Søren Ulstrup[1], Charlotte E. Sanders[1], Jill A. Miwa[1], Deepnarayan Biswas[2], Cephise Cacho[3], Paulina Majchrzak[3], Igor Marković[2], Federico Andreatta[1], Adam Wyatt[3], Marco Bianchi[1], Sanjoy K. Mahatha[1], Luca Bignardi[4], Daniel Lizzit[4], Paolo Lacovig[4], Silvano Lizzit[4], Phil D. C. King[2], and Philip Hofmann[1] — [1]Aarhus University, Aarhus, Denmark — [2]University of St Andrews, St Andrews, UK — [3]Central Laser Facility, Didcot, UK — [4]Elettra Sincrotrone Trieste, Trieste, Italy

The recent development of ultrafast time-resolved photoemission experiments has led to novel findings concerning non-equilibrium electron dynamics. Of particular interest are the 2D semiconducting transition metal dichalcogenides (TMDCs) that can be seen as graphene analogues with strong spin-orbit interactions. Here, the ultrafast dynamics of bilayer MoS_2 on Ag(111) are investigated using time and angle resolved photoemission spectroscopy (TR-ARPES) following an optical excitation with tunable polarisation. Curiously, we find that the nature of the light polarisation dependence for excitation between the valence and conduction bands is different from what would be naively expected on the basis of valley-selection rules. Our results could provide new insight into the interlayer coupling and inter-valley dynamics at play in bilayer TMDCs.

O 12.3 Mon 15:30 MA 005

Ultrafast charge transfer in epitaxial WS_2/graphene van der Waals heterostructures — •Isabella Gierz[1], Sven Aeschlimann[1], Mariana Chavez-Cervantes[1], Razvan Krause[1], Antonio Rossi[2], and Camilla Coletti[2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Nanotechnology @ NEST, Istituto Italiano di Tecnologia, Pisa, Italy

Reduced screening together with confinement results in strong electron-electron interactions in two dimensional solids. Since the discovery of graphene, a semi-metal with linear band structure, many other layered materials have been reduced to monolayer thickness. One example are monolayer group VI transition metal dichalcogenides, direct band gap semiconductors with broken inversion symmetry that, in the presence of strong spin-orbit coupling, produces a sizable spin splitting of the band structure up to several hundreds of meV. Stacking different two-dimensional materials to from van der Waals heterostructures offers the possibility to tune their electronic properties and to produce new functionalities. We use femtosecond laser pulses to photo-dope epitaxial WS_2/graphene heterostructures [1,2] and investigate the resulting carrier dynamics with time- and angle-resolved photoemission spectroscopy (tr-ARPES). We find evidence for ultrafast charge transfer between the layers that rapidly fills the photo-induced holes in the valence band of WS_2.

[1] Rossi et al., 2D Mater. 3, 031013 (2016)

[2] Forti et al., Nanoscale 9, 16412 (2017)

O 12.4 Mon 15:45 MA 005

Ultrafast electron transfer across a ZnO-organic interface — •Lukas Gierster[1], Sesha Vempati[1], Jan-Christoph Deinert[1,2], Anton Zykov[3], Stefan Kowarik[3], Yves Garmshausen[4], Stefan Hecht[4], and Julia Stähler[1] — [1]Fritz-Haber-Institut Berlin, Dpt. Phys. Chem. — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Humboldt-Universität zu Berlin, Dpt. of Physics — [4]Humboldt-Universität zu Berlin, Dpt. of Chemistry

Combining organic molecules with inorganic semiconductors is a promising route towards novel optoelectronic devices, such as organic LEDs or photovoltaics [1]. The electron transfer across the hybrid interface is a crucial factor for the efficiency of such devices. We investigate this fundamental process at the ZnO/p-quinquephenyl pyridine (5P-Py) surface using time-resolved two-photon photoelectron spectroscopy. Upon adsorption of 5P-Py (mass equivalent of 2 ML) on ZnO (10-10) we find an occupied interfacial hybrid state close to the Fermi level. It can be used as an initial state to populate the molecular LUMO without direct excitation of the molecules. The LUMO population decays within 90 fs by electron transfer to ZnO. Furthermore, a bulk 5P-Py film (16 nm) was investigated, which was characterized by AFM and XRD showing a grainy and crystalline structure. Here, excitons were created by HOMO-LUMO excitation, which decay on a picosecond timescale due to exciton diffusion followed by charge separation at the interface as well as recombination. [1] N. Koch, ChemPhysChem 8, 1438-1455 (2007)

O 12.5 Mon 16:00 MA 005

The Unoccupied Electronic Structure of CuPc/PTCDA/Ag(111) Probed with Two-Photon Photoemission — •Klaus Stallberg, Jonas Zimmermann, Alexander Lerch, Andreas Namgalies, and Ulrich Höfer — Fachbereich Physik, Philipps-Universität, D-35032 Marburg

Stacked layers of copper-phthalocyanine (CuPc) and PTCDA on Ag(111) represent a structurally well-defined model for an organic donor-acceptor interface above a metal substrate. The unoccupied electronic structure of this model system is investigated by means of time-resolved two-photon photoemission (2PPE). The 2PPE spectra comprise several photoemission bands which originate from both occupied and unoccupied electronic states. More specifically, we observe direct 2PPE from the CuPc HOMO as well as photoemission involving the n=1 and n=2 image potential states (IPS), a Shockley-derived interface state (IS) at the PTCDA/Ag(111) interface, and excitonic states in the organic heterolayer as intermediate states. Photoemission from the IS is measured for pump photon energies ranging from 1.6 eV to 2.5 eV and is found to follow the optical absorption of CuPc. This indicates efficient transfer of photoexcited electrons from the CuPc layer to the IS at the PTCDA/silver interface which takes place on a timescale of 40 fs. Moreover, we discuss the origin of excitonic bands in the 2PPE spectra and investigate the relaxation dynamics of excitonic states in the CuPc/PTCDA donor-acceptor type heterosystem.

O 12.6 Mon 16:15 MA 005

The role of small polarons in ultrafast electron localization near a model electrolyte/metal interface — •Sarah King, Katharina Broch, and Julia Stähler — Department of Physical Chemistry, Fritz-Haber Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

In the current study, we investigate the formation dynamics of small polarons in thin films of dimethyl sulfoxide (DMSO) near a Cu(111) metal interface using time- and angle-resolved two-photon photoemission spectroscopy. A delocalized electronic state within the second DMSO monolayer is initially formed upon photoexcitation and dynamically becomes a small polaron in DMSO on a 200 fs timescale, consistent with localization due to vibrational dynamics of the DMSO film. The polaron is subsequently further stabilized through longer-range screening on a 600 fs timescale. As the small polaron formation dynamics are the same for both 6 ML and 2 ML of DMSO, the mechanism observed in our experiments is relevant to bulk DMSO near metal surfaces. Furthermore, the small polaron acts as a precursor state for a surface-bound electronic state with a lifetime thirteen orders of magnitude longer. This highlights the way in which electronic states near metal surfaces with femtosecond lifetimes are important precursors for long-lived states of solvents and electrolytes.

15 min. break

Invited Talk O 12.7 Mon 16:45 MA 005

Nonlinear Surface Phonon Polariton Spectroscopy — Nikolai C. Passler[1], Ilya Razdolski[1], Christopher J. Winta[1], Sandy Gewinner[1], Wieland Schöllkopf[1], Stefan A. Maier[2], Joshua D. Caldwell[3], Martin Wolf[1], and •Alexander Paarmann[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Imperial College London, UK — [3]Vanderbilt University, Nashville, USA

There has been much increasing interest recently in the mid-infrared to terahertz spectral response of polar dielectric crystals due to a novel branch of nanophotonics based on surface phonon polaritons (SPhPs) [1], which arise at the surface of these materials due to optical phonon resonances in their dielectric response. Using our in-house free-electron laser [2] as intense and tunable infrared light source, we have developed new approaches of nonlinear solid state spectroscopy, focusing on phonon resonances in polar dielectrics.

Specifically, mid-infrared second harmonic generation (SHG) spectroscopy [3] is used to probe the optical field enhancement associated with resonantly excited SPhPs in sub-diffractional nanostructures [4], as well as prism-coupled propagating SPhPs using the Otto geometry [5]. The latter approach enables mapping of the full SPhP dispersion which can, for instance, reveal the SPhP hybridization in heterostructures.

[1] Caldwell, et al. Nanophotonics 4, 1 (2015) [2] Schöllkopf et al., Proc. SPIE 9512, 95121L (2015) [3] Paarmann, et al. Appl. Phys. Lett. 107, 081101 (2015) [4] Razdolski, et al., Nano Letters 16, 6954 (2016) [5] Passler, et al., ACS Photonics 4, 1048 (2017)

O 12.8 Mon 17:15 MA 005

Ultrafast hot electron dynamics of quantum-well states in momentum space — •Florian Haag[1], Lisa Grad[1], Johannes Seidel[1], Norman Haag[1], Mirko Cinchetti[2], Martin Aeschlimann[1], and Benjamin Stadtmüller[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

Excited electrons play a crucial role for many fundamental chemical and physical phenomena occurring at surfaces, (hybrid) interfaces, or in bulk materials. Here, we use time-resolved 2 photon momentum microscopy to follow the hot electron dynamics in momentum space and to determine the momentum dependent scattering processes of excited electrons.

As model system, we examined the electron dynamics of the quantum-well system Pb on Ag(111) for different laser polarizations and laser fluencies. The momentum dependent hot electron lifetime can be directly correlated to the band dispersion of the QWS. After adsorption of the organic molecule PTCDA, we find an orbital selective hybridization between molecular levels and QWS as well as a significant increase of the momentum dependent electron lifetime throughout the entire momentum space.

O 12.9 Mon 17:30 MA 005

Ultrafast band structure dynamics of thin C_{60} films on Ag(111) — •Sebastian Emmerich[1], Benjamin Stadtmüller[1], Dominik Jungkenn[1], Norman Haag[1], Christina Schott[1], Sebastian Hedwig[1], Steffen Eich[1], Markus Rollinger[1], Mahalingam Maniraj[1], Martin Aeschlimann[1], Mirko Cinchetti[2], and Stefan Mathias[3] — [1]University of Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Physikalisches Institut I, Universität Göttingen, 37077 Göttingen, Germany — [3]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

The performance of organic based electronic devices is determined by the energy level alignment as well as by the excitation dynamics of electrons in these materials. Although both aspects are intrinsically linked by the polarizability of organic materials, they have mainly been discussed separately so far. In this work, we present new insight into the ultrafast band structure dynamics of thin C_{60} films on Ag(111). The combination of time- and angle resolved photoemission with a fs-XUV light source allows us to follow the transient evolution of the unoccupied as well as of occupied band structure after the fs-optical excitation with visible light. The unoccupied part of the C_{60} band structure reveals the well-known quasi-particle dynamics of the exciton formation and its decay in C_{60}. Most interestingly, we observe a transient inhomogeneous broadening of all occupied molecular orbitals upon optical excitation. This effect is attributed to the transient polarization of the molecular film caused by the exciton formation at distinct C_{60} sites.

O 12.10 Mon 17:45 MA 005

Breakdown of the atto-clock concept in attosecond-time-resolved photoemission from solids — •Andreas Gebauer[1,2], Sergej Neb[1], Walter Enns[1], Ulrich Heinzmann[1], Andrey K. Kazansky[3,4,5], and Walter Pfeiffer[1] — [1]Molecular and Surface Physics, University of Bielefeld, Germany — [2]Ultrafast Phenomena At Surfaces, TU Kaiserslautern, Germany — [3]University of the Basque Country, 20080, San Sebastián, Spain — [4]Donostia International Physics Center (DIPC), 20018 San Sebastián, Spain — [5]IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Spain

The availability of single attosecond EUV pulses paved the way to observe electrons at solid surfaces on their natural time scale [1]. In streaking spectroscopy the interaction of a photoelectron with an intense NIR streaking field reveals relative delays of different emission channels with up to 10 as resolution [2].

Here, the impact of an inhomogeneous and penetrating IR field distribution on as-time-resolved photoemission from solid surfaces is simulated based on solving the one-dimensional TDSE [2].

It is shown that the penetration of the IR fields has an substantial impact on the relative delays. Therefore, the phenomenological concept of a classical atto-clock, that can be envisioned as a common finish line for different photoemission channels, needs to be discussed.

[1] A.L. Cavalieri, et al., Nature **449**, 1029 (2007).

[2] F. Siek, et al., Science **357**, 1274 (2017)

O 12.11 Mon 18:00 MA 005

Spin polarization and attosecond time delay in photoemission from condensed matter — •Mauro Fanciulli[1,2], Henrieta Volfová[3], Stefan Muff[1,2], Andrew Weber[1,2], Jan Minár[4], Ulrich Heinzmann[5], and Hugo Dil[1,2] — [1]École Polytechnique Fédérale de Lausanne (CH) — [2]Swiss Light Source, PSI, Villigen (CH) — [3]Ludvig Maximilians Universität München (DE) — [4]University of West Bohemia, Pilsen (CZ) — [5]Universität Bielefeld (DE)

Interfering channels in the photoemission matrix elements are at the origin of spin polarization of the photoelectron beam even when the probed initial state is not spin-polarized [1]. Thus the measurement of spin polarization by means of spin- and angle-resolved photoemission spectroscopy allows to have information on the interference process, and in particular on the phase-shift ϕ_s between the channels. An extension of the Eisenbud-Wigner-Smith (EWS) model of particle scattering allows to relate the attosecond time delay in photoemission to the phase term ϕ of the matrix elements [2].

It will be shown that ϕ is closely related to ϕ_s, and that it is possible to make an indirect estimate of EWS time delays from a (non-time-resolved) spin-resolved experiment [3]. After the description of the model, experimental studies performed at the Swiss Light Source on several condensed matter systems of interest will be presented [3,4].

[1] E. Tamura et al., PRL 59, 08934 (1987) [2] R. Pazourek et al., Rev. of Mod. Phys. 87, 03765 (2015) [3] M. Fanciulli et al., PRL 118, 067402 (2017) [4] M. Fanciulli et al., PRB 95, 245125 (2017)

O 13: Plasmonics and nanooptics: Light-matter interaction, spectroscopy I

Time: Monday 15:00–18:15 Location: MA 041

O 13.1 Mon 15:00 MA 041

Ultrafine-Dust Detection Based on Surface Enhanced Infrared Absorption Using Bowtie Nanoantennas — •Christian Huck[1], Michael Tzschoppe[1], Rostyslav Semenyshyn[2], Frank Neubrech[1], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Heidelberg Universtity, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

In the last years, surface-enhanced infrared absorption (SEIRA) has been established as a powerful method for chemical structure analysis of thin molecular layers. Much less attention has so far been payed to other potential fields of application, such as the detection and characterization of small particles, *e.g.* ultrafine-dust particles. Here, we report on an experimental study, which shows, that deeply subwavelength sized particles can be detected and chemically analyzed by SEIRA. Our study is based on bowtie shaped apertures etched in a thin Au layer, used to enhance phononic excitations[1] of individual silica particles. As it turned out, the bowtie geometry features several advantages for the detection of ultrafine-dust particles, which we want to detail during the talk. Backed up by numerical calculations, we show that a detection limit in terms of a particle diameter of as low as 20 nm can be achieved, corresponding to a ratio to the wavelength of $\lambda^2/d^2 > 250000$. Our approach offers the possibility to analyze infrared vibrations from tiniest particles and thus paves the way toward SEIRA-based fine dust sensing devices.

[1] Huck *et al.* Opt. Express 24, 25528-25539 (2016)

O 13.2 Mon 15:15 MA 041

Continuous-Wave Multiphoton Photoemission from Plasmonic Nanostars — •Murat Sivis[1], Nicolas Pazos-Perez[2], Renwen Yu[3], Ramon Alvarez Puebla[2,4], F. Javier García de Abajo[3,4], and Claus Ropers[1] — [1]4th Physical Institute - Solids and Nanostructures, Georg-August University, Göttingen, Germany — [2]Department of Physical Chemistry and EMaS, Universitat Rovira i Virgili,Tarragona, Spain — [3]Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, Castelldefels, Spain — [4]Institució Catalana de Reserca i Estudis Avançats, Barcelona, Spain

Highly nonlinear optical photoemission from tailored plasmonic nanostructures, as used in localized electron sources, is typically restricted to ultrafast laser pulse excitation due to the required high local intensities. Here, we demonstrate localized 3-photon photoemission from chemically-synthesized plasmonic gold nanostars under continuous-wave illumination at sub-MWcm^{-2} incident intensities. Intensity- and polarization-dependent measurements confirm the nonlinear photoemission from the nanostar tips with feature sizes smaller than 5 nm, which facilitate near-field-intensity enhancement factors exceeding 1000. Our results highlight the possibilities for new designs of nanoscale coherent electron sources, with potential applications in microscopy, spectroscopy and sensing.

O 13.3 Mon 15:30 MA 041

Single Plasmonic Particle Chiral Spectroscopy — •Julian Karst, Mario Hentschel, Nikolai Strohfeldt, and Harald Giessen — 4th Physics Insitute and Research Center SCoPE, University of Stuttgart

Chirality plays a crucial role in our everyday lives. Virtually all studies are performed on large ensembles of chiral objects, which obstructs the contribution of the individual particle. Hence, it is highly desirable to study individual chiral objects. Here, we show that we are able to measure reproducibly circular dichroism spectra in the visible spectral range of left and right handed C4 symmetric single plasmonic oligomer. We utilize darkfield scattering spectroscopy as well as correlative scattering electron microscopy in order to study the influence of structural arrangement and shape on the optical properties of a single plasmonic oligomer. Our two-layered oligomers are fabricated by top-down electron beam lithography to offer a high degree of structural control. We find that even minute structural differences, which we cannot resolve in scanning electron microscopy, manifest themselves in clear differences in the chiroptical response. Our results play an important role for further investigations and optimizations in design, fabrication, and measurements of single plasmonic enantiomers, but also on the way towards single chiral molecule sensing.

O 13.4 Mon 15:45 MA 041

Wavelength-dependent Third Harmonic Generation in Plasmonic Gold Nanoantennas: Role of the d-band — •Joachim Krauth, Mario Hentschel, and Harald Giessen — 4^{th} Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Plasmonic gold nanoantennas are highly efficient nanoscale nonlinear light converters. The nanoantennas provide large resonant light interaction cross sections as well as strongly enhanced local fields. The frequency conversion, however, takes places inside the gold volume and is thus ultimately determined by the microscopic gold nonlinearity. While the influence of the nanoantenna geometry has been studied in great detail, only little attention has been paid to the microscopic material nonlinearity. Here we show that the microscopic third-order nonlinearity of gold is in fact a resonant one by virtue of interband transitions between the d- and sp-bands. Utilizing a large set of resonant nanoantennas and an optical parametric oscillator as broadband tunable light source, we show that the radiated third harmonic (TH) signals significantly increase as soon as the TH becomes resonant with allowed interband transitions. With the help of an anharmonic oscillator model and independent reference measurements on a gold film we can unambiguously demonstrate that the observed TH increase is related to a strongly wavelength-dependent microscopic third-order gold nonlinearity. This additional tuning parameter allows further manipulation and optimization of nonlinear nanoscale systems and thus renders the investigation of other plasmonic materials highly intriguing.

O 13.5 Mon 16:00 MA 041

Nanoscale hydrogenography on individual magnesium nanoparticles — •Florian Sterl, Heiko Linnenbank, Tobias Steinle, Florian Mörz, Nikolai Strohfeldt, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

MgH_2 is considered a promising candidate for solid-state hydrogen storage, owing to its high hydrogen content. It can also be considered a model system for other energy storage materials, such as magnesium-based alloys. While the hydrogen diffusion mechanism in Mg at the 100 μm length scale has been investigated extensively using hydrogenography, in which the optical contrast between a metal and its hydride is exploited, an observation of this process at sub-diffraction limit length scales in single Mg nanoparticles has not been carried out so far.

In order to characterize this process at the nanoscale, we employ scattering type scanning near-field optical microscopy (s-SNOM). In this method, the local scattering ability of a nanoparticle is recorded along with its topography, enabling us to record the local material composition as well as topographical changes during hydrogen absorption and desorption. By combining s-SNOM imaging with dark-field scattering spectroscopy, we observe the distribution of metallic Mg and dielectric MgH_2 during both hydrogen absorption and desorption of Mg nanodisks. Our measurement results indicate a strong influence of the crystallinity, as individual Mg crystallites appear to hydrogenate independently from one another. In the future, this method can also be applied to other hydrogen-storage materials.

O 13.6 Mon 16:15 MA 041

Scanning Tunneling Microscopy Induced Luminescence of Bimodal Exciton-Plasmon Emitters — Pablo Merino[1,3], Anna Rosławska[1], Christoph Grosse[1,4], •Christopher Leon[1], Klaus Kuhnke[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569, Stuttgart, Germany. — [2]Institut de Physique, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland. — [3]present address: Instituto de Ciencia de Materiales de Madrid, CSIC, c/Sor Juana Inés de la Cruz 3, E28049, Madrid, Spain. — [4]present address: Nanophotonics Centre, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom.

Scanning tunneling microscopy induced luminescence (STML) is a unique method to locally excite and observe excitons and plasmons in an electroluminescent material, leading to the implementation of a combined exciton-plasmon light source. The light emission from a proof-of-concept buckyball-based system is characterized at the nanometer scale and the relative contributions of light originating from excitons and plasmons can be reproducibly tuned by STM parameters under exclusion of any tip modification. This ability is intimately related to an understanding of intrinsic properties of excitons and plasmons, namely, their formation and decay mechanisms in conjunction with their associated timescales.

15 min. break

O 13.7 Mon 16:45 MA 041

Localization of photonic modes in optimised disordered amorphous silicon thin films — Martin Aeschlimann[1], •Felix Becker[2], Tobias Brixner[3], Benjamin Frisch[1], Michael Hartelt[1], Matthias Hensen[3], Thomas H. Loeber[4], Walter Pfeiffer[2], Sebastian Pres[3], Bernd Stannowski[5], and Helmut Stiebig[2] — [1]Fachbereich Physik and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern — [2]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld — [3]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [4]Nano-Structuring-Center, Erwin-Schrödinger-Str. 13, 67663 Kaiserslautern — [5]Helmholtz-Zentrum Berlin, PVcomB, Schwarzschildstr. 3, 12489 Berlin

Tailored disordered nanostructures that feature long-living photonic modes are employed to enhance local light scattering, light localization, and absorption. We demonstrate the controlled fabrication of nanotextured a-Si:H absorber layers using focused ion beam milling of planar ZnO substrates and PECVD. This allows studying the light absorption in nanotextured absorber layers with custom designed topographies. Light trapping and absorption in these samples is investigated by time- and energy-resolved PEEM. We observe both, field induced multiphoton photoemission from the scattered light fields in the absorber layer as well as nanolocalized photonic modes featuring highly nonlinear thermionic electron emission. The obtained map of photonic modes and absorption patterns is compared to FTDT simulations.

O 13.8 Mon 17:00 MA 041

Anomalous Kerr effect in hybrid Bi-YIG/Au magneto-plasmonic nanostructures — •Spiridon D. Pappas, Philipp Lang, and Evangelos Th. Papaioannou — Fachbereich Physik und Landesforschungszentrum OPTIMAS, Technische Universität, 67663 Kaiserslautern, Germany

The magneto-optical effects exhibited by ferromagnetic materials can be enhanced by the strong localization of light, enabled by adjacent plasmonic resonances [1,2]. In this work, we reveal the anomalous enhancement of the longitudinal magneto-optical Kerr effect (L-MOKE) in the ferrimagnetic dielectric bismuth substituted yttrium iron garnet (Bi-YIG), induced by localized surface plasmons (LSPs) in gold nanoparticles (AuNPs). In order to reveal the resonant frequency of the LSPs, we used optical spectrophotometry. A Bi-YIG sample containing no nanoparticles was also used as a reference. The magneto-plasmonic response was studied with the aid of a spectroscopic MOKE setup operating in the longitudinal mode, equipped with a filtered supercontinuum laser source. The experimental results reveal an anomalous enhancement of the L-MOKE signal (Kerr rotation, Kerr ellipticity) for the sample containing AuNPs close to the LSP resonances. In order to gain qualitative insight into the mechanism of the exhibited anomalous L-MOKE, the Near Field enhancement close to the LSP frequencies was simulated computationally.

[1] V. I. Belotelov et al., Nat. Nanotechnol. 6, 370 (2011).

[2] M. Rollinger et al., Nano Lett. 16, 2432 (2016).

O 13.9 Mon 17:15 MA 041

Visualization of photoemission quantum pathways via photon-plasmon spin-orbit mixing — •Eva Prinz[1], Grisha Spektor[2], Deirdre Kilbane[3], Anna-Katharina Mahro[1], Michael Hartelt[1], Meir Orenstein[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Department of Electrical Engineering, Technion - Israel Institute of Technology, Israel — [3]School of Physics, University College of Dublin, Ireland

Transformation of light carrying spin angular momentum (SAM) to an optical field vortex carrying angular momentum (OAM) has been of wide interest in recent years [1]. We measured the interaction between 3D light carrying axial SAM and 2D plasmon-polariton vortices carrying high order transverse OAM [2].

The interaction is mediated via two-photon absorption on a gold surface, imprinting the resulting angular momentum mixing into matter by excitation of electrons that are photo-emitted into vacuum and detected by PEEM. We show experimentally and theoretically that the absorptive nature of this interaction leads to both single and double photon-plasmon angular momentum mixing processes which correspond to different quantum pathways of the electron excitation.

[1] Bliokh et al., Nature Photonics 9 (2015)

[2] Spektor et al., Science 355 (2017)

O 13.10 Mon 17:30 MA 041

Electron-induced photon emission above the quantum cutoff due to time-energy uncertainty — •Kira Kolpatzeck, Philip Kapitza, Ebru Ekici, Christian A. Bobisch, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

We have studied the light emission resulting from inelastic tunneling processes in the tip/sample junction between a silver covered PtIr tip and an Ag(111) surface with a low-temperature scanning tunneling microscope at 80 K. The observed light emission between the visible and the near infrared range carries information about the underlying inelastic processes. It has been studied around the cutoff at $h\nu = eV_\mathrm{T}$.

A detailed analysis of the emission spectra normalized to a reference spectrum recorded at high voltages shows emission tails exceeding the energy eV_T provided by the the applied voltage V_T. For a satisfying explanation the consideration of thermal broadening of the electron Fermi distribution is insufficient. However, a correct description is found if a finite lifetime of the excited states in the range of 30-80 fs, causing a natural linewidth broadening, is included [1].

[1] E. Ekici, P.Kapitza, C. A. Bobisch, R. Möller, Opt. Lett. 42, 4585-4588 (2017).

O 13.11 Mon 17:45 MA 041

Measuring the Orbital Angular Momentum of Plasmonic Vortex Fields — •Pascal Dreher[1], David Janoschka[1], Norman Dünne[1], Bettina Frank[2], Timothy J. Davis[2,3], Harald Giessen[2], Michael Horn-von Hoegen[1], and Frank Meyer zu Heringdorf[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [2]4th Physics Institute and Stuttgart Center of Photonics Engineering (SCoPE), University of Stuttgart, Stuttgart, Germany — [3]School of Physics, University of Melbourne, Parkville, Victoria, Australia

The ability of light to carry orbital angular momentum in addition to its spin angular momentum has been thoroughly investigated in the past. Recent efforts have shown that the combination of these angular momenta can be utilized to excite surface plasmon polaritons with helical wavefronts, i.e. plasmonic vortices. The angular momentum of the exciting light is completely transferred to the plasmon. Further angular momentum can be transferred to the plasmonic field in the form of a topological charge provided by helical nanostructures, e.g. Archimedean spirals. We will report on the imaging of plasmonic vortex fields employing pump-probe photoemission electron microscopy (PEEM) with sub-femtosecond time resolution. We show that the angular momentum state of plasmonic vortices can be extracted from time-integrated PEEM micrographs, by analyzing the plasmonic field distribution for Archimedean spirals with topological charges from one to ten. The presented results agree with the predictions of the Bessel theory for plasmonic vortices.

O 13.12 Mon 18:00 MA 041

Circular dichroism in laser induced electron emission from metallic nanohelixarrays — •Daniel Nürenberg[1], Andrew G. Mark[2], Peer Fischer[2], and Helmut Zacharias[1] — [1]Physikalisches Institut & Center For Soft Nanoscience, Münster, Germany — [2]Max Plank Institut für intelligente Systeme,Stuttgart, Germany

We investigate the electron emission from metallic nanohelices on silicon triggered by fs laser radiation from an optical parametric chirped pulse amplifier. We find a strong asymmetry regarding to left and right circularly polarized excitation in the electron yield in accordance to the handedness of the helices. The emission can be interpreted in terms of a non-equilibrium heating of the electron gas by surface plasmon excitation. Simulations of the surface plasmons correlate the polarization dependence of the photosignal to the local field enhancement on the nanostructures.

O 14: Organic-inorganic hybrid systems and organic films II

Time: Monday 15:00–18:15 Location: MA 042

Invited Talk O 14.1 Mon 15:00 MA 042

Non-commensurate epitaxy with and without coincidences — •Roman Forker — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

The self assembly of atoms or molecules at surfaces is governed by the balance between adsorbate–adsorbate and adsorbate–substrate interactions. Energetic minimization may be achieved through different types of epitaxy. Besides the well-known commensurate registries there are also the less familiar “on-line coincidences”, where the surface unit cells of the adsorbate and of the substrate have a common periodicity in one direction only [1]. Recently, highly ordered molecular monolayers were found to be room-temperature-stable even in the absence of any coincidence with the substrate Hence, the concept of lattice epitaxy fails to explain the evident energy minimum in such a case. Instead, we found that stabilization occurs through so-called static distortion waves that manifest in measurable sub-Ångström lateral shifts away from the positions of a translationally symmetric lattice (which itself is incommensurate) [2]. In the talk I will classify epitaxy using an easy-to-grasp scheme applicable both in reciprocal space and in real space. Several instructive literature examples of experimental structural characterization using scaning tunneling microscopy (STM) and low-energy electron diffraction (LEED) will be elaborated. The ultimate goal is to emphasize the importance of non-commensurate overlayer structures for the systematic understanding of epitaxy.

[1] R. Forker *et al.*, Soft Matter **13**, 1748 (2017).

[2] M. Meissner *et al.*, ACS Nano **10**, 6474 (2016).

O 14.2 Mon 15:30 MA 042

Electrospray deposition of P3HT on Au(110): An STM study — •Theresa Simon[1], Erik Schreck[1], Stefan Förster[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

In the course of characterizing the structure of polymers in contact with solid surfaces, the adsorption of Poly(3-hexylthiophene) (P3HT) on Au(001) [1] leads to a 2D random coil like chain configuration but also molecules in straight *all-trans* geometry are found.

Here we present the investigation of P3HT on the (2 x 1)-missing-row reconstructed Au(110) surface, which provides a stronger 1D template for polymere adsorption. *In situ* scanning tunneling microscopy reveals molecular P3HT chains which are constraint into a fully stretched configuration along the $[\bar{1}10]$ and [001] high symmetry directions indicating a strong molecule-substrate interaction. Chains parallel to the $[\bar{1}10]$ direction are embedded into the surface by the removal of one or two Au reconstruction rows. Beside these straight polymer sections also polymers aligned in the [001] direction or under discrete angles with respect to the surface reconstruction are present together with a minority in random coil configuration.

[1] Förster et al., JCP 141(2014)054713

O 14.3 Mon 15:45 MA 042

Oligomers on nanostructured surfaces: Adsorption-induced alteration of the surface reconstruction — •Laura Katharina Scarbath-Evers[1], Milica Todorović[2], René Hammer[1], Wolf Widdra[1], Daniel Sebastiani[1], and Patrick Rinke[2] — [1]Faculty of Natural Sciences II, Martin-Luther University, Halle-Wittenberg — [2]Department of Applied Physics, Aalto University, Finland

Theoretical studies of organic adsorbates on metal surfaces have mainly focused on the adsorption of small molecules on ideal surfaces. However, many surfaces, e.g. low index surfaces of Au, Ir, and Pt, have complex reconstructions that are challenging for surface science studies. In this work, we approach such complex (or nano-structured) surfaces with a combination of density-functional theory (DFT) calculations and scanning tunnelling microscopy (STM) measurements for the example of the α-sexithiophene (α-6T) oligomer adsorbed on the reconstructed Au(100) surface. We find that due to its corrugation pattern the reconstructed Au(100) surface offers a wide range of adsorption sites than can be broadly classified into *on-ridge* and *in-valley* types with energetic adsorption preferences for the latter. Surprisingly, adsorption in energetically ill-favored *on-ridge* positions leads to strong alterations of the surface reconstruction, facilitated by the “soft” nature of gold. As a result of electrostatic effects and charge transfer between the surface and the molecule, α-sexithiophene displaces the ridge instead of migrating into the valley.

O 14.4 Mon 16:00 MA 042

Adsorption and Monolayer Formation of Sexiphenyl on In_2O_3(111) investigated with STM/AFM — •Margareta Wagner[1], Jakob Hofinger[1], Martin Setvín[1], Lynn A. Boatner[2], Michael Schmid[1], and Ulrike Diebold[1] — [1]TU Wien, Austria — [2]Oak Ridge National Laboratory, USA

The performance of an organic-semiconductor device is critically determined by the geometric alignment, orientation, and order of the organic molecules. While an organic multilayer eventually adopts the crystal structure of the organic material, the interface with the substrate/electrode material is often less well-defined. This work focuses on the prototypical organic molecule para-sexiphenyl (6P) and the thermodynamically most stable surface of the most-common transparent conducting oxide, indium (tin) oxide, $In_2O_3(111)$. The onset of nucleation and the formation of the first monolayer are followed with scanning tunneling microscopy (STM) and constant-height non-contact atomic force microscopy (nc-AFM). At room temperature, 6P adsorbs lying on the surface and randomly oriented, i.e., without an ordered structure. Annealing to 200 °C provides sufficient thermal energy for the molecules to orient themselves along the high-symmetry directions of the surface, leading to a single adsorption site. With increasing coverage, the 6P molecules first form a lose network with poor long-range order but eventually the molecules re-orient and the first monolayer is established. It is a densely-packed, well-ordered (1×2) structure with one 6P per $In_2O_3(111)$ substrate unit cell.

O 14.5 Mon 16:15 MA 042

Investigation of Caffeine Monolayer Formation on Au(111) — •Malte Schulte, Adam Budde, Ismail Baltaci, Peter Roese, and Carsten Westphal — Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Straße 4a, 44227 Dortmund, Germany

Research on self-assembled molecules on metal surfaces has attracted strong interest in the last few years. Additionally, different phases and polymorph behavior of molecules is in the focus especially for pharmaceutical studies. Caffeine is a psychoactive drug and solid caffeine molecules show polymorph behavior with a stable β and a metastable high-temperature α phase. In order to study these aspects from a bottom-up approach we deposited caffeine molecules on an Au(111) surface under ultra-high vacuum conditions. We investigated monolayer self-assembly of caffeine molecules on the surface with scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) and observed different orientations of the caffeine molecules on the substrate.

15 min. break

O 14.6 Mon 16:45 MA 042

Contact formation at organic-inorganic interfaces — •Steffen Duhm — Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, China

Conductivities in organic semiconductor thin films are notoriously low and engineering injections barriers at active layer-electrode interfaces is a successful approach to increase charge carrier concentrations. Strongly coupled organic-metal interfaces involve charge transfer and hybridization and vertical bonding distances and adsorption induced molecular distortions are crucial for the energy-level alignment and thus for the charge injection properties at these interfaces. Element-specific bonding distances of organic (sub)monolayers on the (111)-surfaces of coinage metals have been measured by the X-ray standing wave (XSW) technique. Interface energetics and chemical reactions have been accessed by ultraviolet photoelectron spectroscopy (UPS) and X-ray photoelectron spectroscopy (XPS). By increasing the complexity of the systems from pure hydrocarbon systems like pentacene or perylene to oxygen and/or nitrogen substituted derivatives we could identify the pivotal role of these side-groups in the process of surface-induced aromatic stabilization, which results in metallic organic monolayers.

O 14.7 Mon 17:00 MA 042

Monitoring ligand induced assembly of PbS nanocrystals on the liquid surface by in-situ grazing incidence X-ray scattering — •Santanu Maiti[1], Sonam Maiti[1,2], Jan Hagenlocher[1], Andre Maier[2], Andrei Chumakov[3], Marcus Scheele[2], and Frank Schreiber[1] — [1]Institute of Applied Physics, University of Tuebingen, Auf der Morgenstelle 10, 72076 Tuebingen, Germany — [2]Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 18, 72076 Tübingen, Germany — [3]ID10, European Synchrotron Radiation Facility (ESRF), 38000 Grenoble, France

Hybrid nanostructures, composed of inorganic nanocrystals (NCs) and organic semiconductor (OSC) molecules exhibit efficient charge transport and optoelectronic properties[1,2]. The OSC ligand (CuTAPc) induced structural evolution and growth kinetics of PbS NC superlattices at the acetonitrile/air interface has been monitored by in-situ grazing incidence small angle X-ray scattering and grazing incidence X-ray diffraction in real time[3-4]. A continuous in-plane contraction of the superlattice monolayer with time and an overall shrinkage of 5% in lattice constant after complete exchange has been observed. In addition, the atomic orientation of the NCs has been figured out during the exchange process. The combined results provide a complete understanding of atomic and nano-scale assembly of NCs during ligand exchange. 1. M. P. Boneschanscher et al., Science 344, 1377 (2014); 2. M. Scheele et al., PCCP 17, 97 (2015); 3. S. Maiti et al., JPCM, 29, 095101 (2017); 4. A. Andre et al., Chem. Mater. 27, 8105 (2015).

Invited Talk O 14.8 Mon 17:15 MA 042

Spotlight on Excitonic Coupling in Textured and Polymorphic Anilino Squaraine Thin Films — •Manuela Schiek — Institute of Physics, University of Oldenburg, Germany

Squaraines are small molecular quadrupolar donor-acceptor-donor (D-A-D) chromophores absorbing in the red spectral range considered for application as photovoltaic materials [1, 2]. A prototypical anilino squaraine with branched alkyl side chains (SQIB) crystallizes into two polymorphic bulk structures with different intermolecular interaction schemes. However, both crystal phases support Davydov splitting and thus show pleochroic absorbance spectra. In spin-casted [3] and vapor deposited [4] thin films X-ray diffraction probes these two phases with a strongly preferred out-of-plane orientation directed by the annealing temperature or by the choice of growth substrate, respectively. Linear polarized spectro-microscopy recordings locate the spatial orientation of the transition dipole moments and allow assignment of the Davydov components. Combined with cross-polarized and atomic force microscopy we obtain a complete picture of molecular orientation and excitonic coupling within the distinct morphological features and relative to the substrate [3].
[1] D. Scheunemann et al., Appl. Phys. Lett. 111 (2017) 183502. [2] O.S. Abdullaeva, A. Lützen, K. Dedek et al., Langmuir 32 (2016) 8533. [3] F. Balzer, M. Silies, C. Lienau et al., Cryst. Growth Des. (2017) DOI: 10.1021/acs.cgd.7b01131. [4] T. Breuer, G. Witte et al., unpublished results.

O 14.9 Mon 17:45 MA 042

Adsorption of squaraine molecules to Au(111) and Ag(001): Role of the substrate symmetry — •Maike Luft, Boris Gross, Manuela Schiek, and Niklas Nilius — Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany

The adsorption of squaraines, an important chromophore for the use in organic solar cells, to Ag(001) and Au(111) is studied with STM. Self-assembly into square building blocks is revealed on Ag(001), while no long-range order is observed on Au(111). Squaraine binding to Ag is mediated by carbonyl-oxygen and hydroxyl groups located in the molecular center, while hydrogen bonding between the terminal isobutyl groups and the oxygen species governs the intermolecular coupling. The latter is maximized by rotating the molecules by a few degrees against a perfect square orientation. On Au(111), no squared molecular network forms due to symmetry reasons. Moreover, the high electronegativity of gold reduces the directing effect of oxygen-metal bonds that control the ordering process on Ag. As a result, only frustrated three-fold symmetric molecular units but no extended network develops on Au(111).

O 14.10 Mon 18:00 MA 042

Azulene and naphthalene: two isomers with different adsorption on metal surfaces — •Juliana Morbec and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany

Azulene and naphthalene have the same molecular formula ($C_{10}H_8$) but different motifs and different electronic properties. Naphthalene has a regular 6-6 motif, with two hexagons, while azulene has a pentagon and a heptagon (5-7 motif). The non-alternant topology of azulene and the absence of mirror-related molecular orbitals lead to significant differences in its electronic structure when compared to naphthalene; in particular, azulene exhibits non-uniform charge distribution, more localized frontier orbitals, large in-plane dipole moment and blue color. Here, we present a first-principles study of the adsorption of these isomers on the Ag(111) and Cu(111) surfaces. We show that azulene interacts more strongly with the metal surfaces than naphthalene. On Cu(111), in particular, azulene presents a significantly larger adsorption energy (by a factor of 2) and larger deformation than naphthalene; analyses of the density of states show that the molecular features of azulene completely disappear upon adsorption on Cu(111), indicating a chemisorption process. We will compare our results with data obtained from NIXSW and TPD measurements.

O 15: Graphen: Adsorption, intercalation and doping I (joint session O/TT)

Time: Monday 15:00–16:30 Location: MA 043

O 15.1 Mon 15:00 MA 043

Intercalation of epitaxial graphene: possible mechanisms — •Mikolaj Lewandowski[1], Ewa Madej[2], Zygmunt Milosz[1], Dorota Wilgocka-Slezak[2], Michal Hermanowicz[3], Nika Spiridis[2], Jozef Korecki[2], Stefan Jurga[1], and Feliks Stobiecki[1] — [1]NanoBioMedical Centre, Adam Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland — [2]Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Niezapominajek 8, 30-239 Krakow, Poland — [3]Institute of Physics, Poznań University of Technology, Piotrowo 3, 60-965 Poznan, Poland

Intercalation of epitaxial graphene (EG) with atoms of various elements may modify EG's structure and electronic properties, which is related both to the weakening of the graphene-support interaction, as well as the interaction of graphene with the intercalated material. We used scanning tunneling microscopy (STM), low energy electron microscopy (LEEM) and low energy electron diffraction (LEED) to study the mechanisms of intercalation of epitaxial graphene (EG) grown on Ru(0001) by thermal decomposition of ethylene (C_2H_4). The results revealed direct influence of graphene's preparation method on its structure and the intercalation mechanisms. The experimental results were supported by theoretical ab initio calculations.

Acknowledgment: The work was financially supported by the National Science Centre of Poland (OPUS project No. 2014/15/B/ST3/02927).

O 15.2 Mon 15:15 MA 043

Modification of the graphene/SiC(0001) interface by intercalation of antimony — •Susanne Wolff[1], Florian Speck[1], Martina Wanke[1], Felix Timmermann[2], Manfred Albrecht[2], and Thomas Seyller[1] — [1]Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany — [2]Lehrstuhl für Experimentalphysik IV, Universität Augsburg, Universitätsstr. 1 Nord, D-86159 Augsburg, Germany

Sublimation growth of graphene on SiC(0001) in argon atmosphere is a well-established method for the preparation of graphene. The first grown carbon layer is partially covalently bound to the Si atoms of the substrate. This so-called buffer layer lacks the electronic properties of graphene. A decoupling of the buffer layer from the SiC substrate can be achieved by intercalation, resulting in quasi-freestanding graphene, with electronic properties tuned by the choice of the intercalant.

We use x-ray photoelectron spectroscopy and angle-resolved photoelectron spectroscopy to investigate the intercalation of antimony. Antimony was deposited on the buffer layer by molecular beam epitaxy. Subsequent annealing in argon at atmospheric pressure results in an intercalation of metallic and oxidized antimony. A pre-intercalation annealing in argon enables an intercalation of metallic antimony only, resulting in a moderate n-type doping of the quasi-freestanding graphene.

O 15.3 Mon 15:30 MA 043

Sulfur intercalation underneath single-layer graphene on Ru(0001) — •Lars Buss[1], Moritz Ewert[1,2], Jens Falta[1,2], and Jan Ingo Flege[1,2] — [1]Institute for Solid State Physics, University of Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Germany

The strong binding of epitaxially grown single-layer graphene to a wide range of transition metals has detrimental influence on its electronic properties. However, by lifting the interlayer coupling, e. g., via intercalation routes, its unique electronic properties can be restored. We have investigated the interaction of sulfur with single-layer graphene grown on Ru(0001) by ethylene exposure under UHV conditions with *in situ* low-energy electron microscopy (LEEM) and micro-diffraction (μLEED). At elevated temperature and under dimethyl disulfide background pressure, we observe that sulfur intercalates through the open edges of the graphene islands and proceeds along the substrate steps. Prolonged exposure to sulfur is also seen to induce cracking of the graphene islands perpendicular to the substrate steps, consistent with substantial relief of tensile strain after successful sulfur insertion underneath the graphene. This interpretation is backed by μLEED patterns collected from single graphene islands that consist of an incoherent superposition of the LEED patterns observed individually for pure graphene as well as pure sulfur adsorption on the clean Ru surface, indicating that the graphene layer is virtually decoupled from the substrate.

O 15.4 Mon 15:45 MA 043

Photoemission study of the intercalation of transition metals underneath graphene on silicon carbide — •Richard Hönig, Philipp Espeter, Peter Roese, Karim Shamout, Ulf Berges, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Strasse 4a, 44227 Dortmund, Germany

Silicon carbide (SiC) is among the most promising substrates on the route to real-life graphene (G) applications. While the basic properties of G/SiC were well elucidated during the past decade, present research is focused on G/SiC as a building block of multilayer systems. In our study we analyze the interaction of G/SiC with magnetic transition metals in order to explore the potential for spintronic applications. Here, cobalt and nickel are most interesting due to a well-matched lattice constant.

The 6H-SiC(0001) samples are prepared by annealing in argon gas at atmospheric pressure leading to large-area growth. Then the sample is covered with thin transition metal films with thicknesses up to a few nanometers. Our main characterization methods are threshold photoemission electron microscopy (PEEM) and synchrotron based photoelectron spectroscopy (PES).

We performed a film thickness and temperature dependent study for Co on G/SiC and will present series of PEEM images acquired during in-situ sample annealing. Furthermore, on the basis of PES spectra we discuss the electronic structure of our sample system. Finally, we are looking forward to present first PEEM images of this sample system acquired with circularly polarized soft x-rays.

O 15.5 Mon 16:00 MA 043

Decoupling of the graphene/ferromagnet interface by gold intercalation: Effect on optical constants — •Christine Jansing[1], Hans-Christoph Mertins[1], Markus Gilbert[1], Maxim Krivenkov[2], Andrei Varykhalov[2], Oliver Rader[2], Andreas Gaupp[2], Andrey Sokolov[2], Hud Wahab[3], Heiko Timmers[3], Dominik Legut[4], and Peter M. Oppeneer[5] — [1]Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert Einstein Str. 15, D-12489 Berlin — [3]University of New South Wales, Canberra, ACT 2600, Australia — [4]IT4Innovations Center, VSB-Technical University of Ostrava, CZ-708 33 Ostrava, Czech Republic — [5]Department of Physics and Astronomy, Uppsala University, S-75120 Uppsala, Sweden

X-ray absorption and reflectance spectroscopy of linearly polarized synchrotron radiation across the carbon 1s edge of graphene/Co/W and graphene/Ni/W is utilized to investigate the effect of gold intercalation on the complex optical constants of these systems. The p_z-orbitals of graphene hybridize strongly with the $3d$ states of the ferromagnetic substrate. Hybridization effects can be reduced by intercalation of gold which also leads to a change in the optical constants. A complete set of optical constants was determined, describing the π^*- and σ^*- resonances of graphene. The absorption index k was directly deduced from the measured absorption spectra whereas the refractive index n has been extracted from k via a Kramers-Kronig transformation. Based on these optical constants reflection spectra have been simulated that are in good agreement with our experimental data.

O 15.6 Mon 16:15 MA 043

Graphene protected surface state on Ir(111) with adsorbed lithium — •Predrag Lazic[1] and Petar Pervan[2] — [1]Rudjer Boskovic Institute, Zagreb, Croatia — [2]Institute of Physics, Zagreb, Croatia

It is well known that electronic surface states get strongly perturbed upon the chemical adsorption of very small amount of adsorbates. Adsorption of lithium atoms on Ir(111) is no expection to that rule. Iridium surface state get strongly perturbed and is practically eradicated - it can not be seen as a sharp peak in the ARPES measurement. However, if the graphene is added on top of Ir/Li system the iridum surface state magically reapears. We present a combined experimental and theoretical study of the described system. Using the density funcional theory calculations for large unit cells with disordered lithium atoms geometries on the (111) surface of iridium we were able to reproduce the results of the ARPES measurements -showing clearly that the surface state signal is strongly suppresed when lithium is adsorbed, while it is almost unchanged when lithium is intercalated (i.e. with graphene on top of it). Looking at the projected density of states we constructed a rather simple model explaining this behavior which seems to be general.

O 16: Heterogeneous Catalysis: Theory

Time: Monday 15:00–18:15 Location: MA 141

O 16.1 Mon 15:00 MA 141

The devil is in the defects: first-principles modeling of oxide formation at Pd(100) — •ALBERT BRUIX and KARSTEN REUTER — Technical University Munich

The surfaces of many late transition metals are oxidized under ambient conditions or at increased oxygen pressures, which has strong implications for corrosion and catalysis. Stable O-enriched states resulting from oxidation may consist of the metal surface with high concentration of adsorbed O atoms, the corresponding metal-oxide, or something in between (e.g. surface oxides). A quantitative atomistic modeling of oxidation reactions catalyzed on transition metals therefore requires an understanding of the properties and formation mechanisms of the oxidized surfaces. In this work, the oxidation of Pd(100) to the corresponding surface oxide phase PdO(101)/Pd(100) formed on it is addressed by means of Density Functional Theory calculations. We focus on the oxidation mechanisms involving the pristine metal surface and different surface defects. The under-coordinated sites at surface steps, kinks, and small clusters or islands are found to play an important role in the oxidation process, affecting both the initial adsorption of oxygen and the transformation to the surface oxide phase.

O 16.2 Mon 15:15 MA 141

Insights into the Relative Importance of Ripening and Particle Migration for Sintering of Pt Nanoparticles — •ELISABETH DIETZE[1], FRANK ABILD-PEDERSEN[2], and PHILIPP N. PLESSOW[1] — [1]Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Stanford, USA

A rational approach to improve the stability of heterogeneous transition metal catalysts requires to understand deactivation mechanisms on an atomic scale. For Pt nanoparticles, simulations have shown that ripening through the gas phase via volatile PtO_2 is relevant for sintering [1], but surface migration could not be excluded as an alternative mechanism. Recently, the migration of Pt particles was modeled from first principles [2] and diffusion constants were extracted. Using these diffusion constants, the importance of particle migration for sintering can now be estimated. To model the position and migration of particles, we use a kinetic Monte Carlo rather than a mean field model. This also allows us to explicitly study the effect of defects. The developed approach is able to simulate both ripening and particle migration and one can therefore compare the relative importance of these two mechanisms. We furthermore investigate how temperature, partial pressure of oxygen, binding strength of defects and the shape of the PSD influence the sintering kinetics.

References: [1] Plessow, P. N.; Abild-Pedersen, F., ACS Catal. 2016, 6 (10). [2] Li, L., et al. J. Phys. Chem. C 2017, 121(8).

O 16.3 Mon 15:30 MA 141

Steps and catalytic reactions: First-principles Kinetic Monte Carlo study on CO oxidation with preadsorbed O on Rh (553) — •BAOCHANG WANG[1], CHU ZHANG[2], JOHAN GUSTAFSON[2], and ANDERS HELLMAN[1] — [1]Department of Physics and the Competence Centre for Catalysis, Chalmers University of Technology, 41296, Sweden — [2]Synchrotron Radiation Research, Lund University, Box 118, 221 00 Lund, Sweden

Many catalytic reactions display strong structure sensitivity, and particular steps and defects are often identified as active sites for the reactions at hand. A controlled way to address this is to use vicinal surfaces where the step density is known. Here we studied the CO oxidation reaction on oxidized Rh(111) and Rh(553) by first-principles methods coupled with Kinetic Monte Carlo (KMC) to provide insight to the structure sensitivity on Rh. Our recent experiment shows that the reaction between CO and preadsorbed O proceeds at lower temperature on a stepped Rh(553) surface than on a flat Rh(111), indicating that stepped surfaces are more catalytically active. After removing half of the oxygen, however, the reaction slows down significantly and the O coverage seem to remain as 25% of the initial coverage. First-principles calculations were performed to investigate the different possible reaction pathways on the surfaces. A lattice KMC model was built based on the calculated barriers. We do, however, find that this is not thanks to reactions on the steps, but rather on the terraces close to the steps. Our theory results are compared to experimental data, both concerning the CO activity but also core-level spectroscopy.

O 16.4 Mon 15:45 MA 141

Finite-Temperture Statistical Study of Small Silver Clusters Ag_n (n= 4-13) interacting with O_2 molecules — •WEIQI WANG and LUCA M. GHIRINGHELLI — Fritz-Haber-Institut der MPG, Berlin

Due to their unique physical and chemical properties, noble-metal clusters have attracted tremendous interest in recent decades. In this work, we systematically study both the static and the dynamical properties at finite temperature of sub-nanometer-sized neutral silver clusters Ag_n (n= 4-13), with and without adsorbed O_2, in order to reveal correlations between the structure, the local charge, and the bond dynamics.

Clusters with different (fixed) spin states are sampled at different temperatures by replica-exchange *ab initio* molecular dynamics, where the forces bewteen atoms are described via density-functional theory.

Regarding dynamical properties, we focus our attention on the bond life-time, studied by means of the bond auto-correlation function.

Interestingly, we find a correlation between the local charge state of bonded atom pairs, estimated via the Hirschfeld charge partitioning, and the bond life-time. In particular, negatively charged Ag binded pairs (with elongated Ag–Ag bond) tend to have shorter bond life times. Since O_2 molecules tend to adsorb onto these negatively charged sites, the O–O bond gets activated upon adsorption. This suggests that the local charge may be a good descriptor for the identification of active sites on the nanoclusters.

O 16.5 Mon 16:00 MA 141

Ethanol dehydrogenation and oxygen dissociation on the Ni- and Rh-doped Au(111) surface — •OZAN DERNEK[1], HANDE ÜSTÜNEL[1], and DANIELE TOFFOLI[2] — [1]Department of Physics, Middle East Technical Univesity, Dumlupinar Boulevard 1, 06800, Ankara, Turkey — [2]Dipartimento di Scienze Chimiche e Farmaceutiche, Universita degli Studi de Trieste Via L. Giorgieri 1 , I-34127, Trieste, Italy

The byproducts of the combustion reaction of alcohols find uses in a wide range of applications in food, pharmaceutical, polymer and plating industries along with many others. As a result, there are considerable economical interests in the design of efficient, low-cost and environmentally low-impact synthetic routes of these products.

The aim of this study is to design Au surfaces by means of doping the surface with Ni and Rh atoms in low concentrations to increase the performance of the surface for selective oxidation of ethanol and dissociation of O_2. We utilize arguably the most successful theoretical method to ever have been used in surface science, namely Density Functional Theory (DFT), to understand the selective oxidation of ethanol and dissociation of O_2 to atomic oxygen. We present the the reaction pathways and activation barriers for both reactions.

This work is supported by TÜBİTAK (The Science and Technological Research Council of Turkey)(Grant no:113F099).

O 16.6 Mon 16:15 MA 141

Promotoreffekt von Alkalimetallen bei Epoxidation von Ethylen über Silberkatalysatoren — •MATEJ HUŠ und ANDERS HELLMAN — Fakultät für Physik, Technische Hochschule Chalmers, SE-41296 Göteborg, Schweden

Die Oxidation von Ethylen zu Epoxiden ist eine der wichtigsten Reaktionen in der chemischen Industrie. Im industriellen Maßstab werden üblicherweise Silberkatalysatoren verwendet. Zur Vermeidung der vollständigen Oxidation zu CO_2 muss CsCl als Promotor beigemischt werden. Der Mechanismus, welcher zu einer Erhöhung der Selektivität führt, ist umstritten. Basierend auf Dichtefunktionaltheorie-Rechnungen haben wir den Einfluss der Alkalimetalle auf die Selektivität untersucht. Unsere Rechnungen zeigen, dass alle Alkalimetalle die Selektivität signifikant erhöhen während die Aktivität des Katalysator reduziert wird. Der Effekt ist umso ausgeprägter je elektropositiver das Alkalimetall. Die Ursache für die Erhöhung der Selektivität und Absenkung der Aktivität ist ein durch die Alkalimetalle auf der Katalysatoroberfläche induziertes elektrisches Feld. Durch die Beimischung von Cl kann die Aktvität ohne Verlust von Selektivität wieder hergestellt werden. Unsere Rechnungen zeigen, dass die Kombination von elektronegativem Cl und elektropositivem Cs einen optimalen Kompromiss aus Aktivität und Selektivität bietet.

15 min. break

O 16.7 Mon 16:45 MA 141

Cheap and Accurate Descriptors for the Computational Screening of Bimetallic Catalysts Identified Using Compressed-Sensing — •Mie Andersen[1], Sergey V. Levchenko[2], Matthias Scheffler[2], and Karsten Reuter[1] — [1]Theoretical Chemistry, Technische Universität München, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Computational screening for new and improved catalyst materials requires cheap and accurate descriptors for energy trends in surface adsorption. To this end, simple and intuitive physical models such as the *d*-band model or scaling relations have proven highly successful for transition metal catalysts [1]. Here we apply SISSO [2], a recently developed compressed-sensing method, to identify more accurate descriptors for surface adsorption using a training data set of adsorption energies of atomic and molecular adsorbates on the fcc(211) facets of elemental transition metals. The descriptors are constructed as nonlinear functions of primary features, which can be obtained at low computational cost from the clean metal surface. Examples of primary features are *d*- and *sp*-projected density of states at the Fermi level, *d*-band filling, *d*-band center, and the Pauling electronegativity of the metal atom. We illustrate the superior predictive performance of the found descriptors on a test data set of adsorption energies on alloy surfaces and apply the new model to the computational screening of bimetallic catalysts for methanol synthesis.

[1] F. Abild-Pedersen, Catal. Today **272**, 6 (2016)

[2] R. Ouyang *et al.*, arXiv:1710.03319

O 16.8 Mon 17:00 MA 141

Evaluation of the Density Functional based Tight Binding method for the study of graphene nucleation on Cu catalysts — •Juan Santiago Cingolani, Mattia Peluchetti, Mie Andersen, and Karsten Reuter — Chair of Theoretical Chemistry, Technische Universität München, Germany

Graphene nucleation on a liquid Cu surface has been shown to produce uniform monolayer continuous films [1] and thus has gained attention in recent years. Molecular dynamics (MD) simulations could provide insights into the processes involved, but the system sizes and timescales required lie outside of the scope of Density Functional Theory (DFT) methods. The Density Functional based Tight Binding (DFTB) method, which provides a significant speedup while retaining a reasonable accuracy, could prove to be a viable alternative. We evaluate the performance of a set of DFTB parameters developed by Li et al [2] by making a series of calculations on the interaction of C atoms on a Cu (111) surface and comparing these results with literature DFT data. We then benchmark selected snapshots from DFTB-driven MD simulations against DFT. Remarkably, reaction and activation energies for monomer diffusion and C-C nucleation are reproduced within 0.1 eV. While our results are promising, further benchmarks against experimental data need to be carried out to validate the use of DFTB in the study of graphene nucleation on molten Cu surfaces.

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

[2] H.-B. Li, A. J. Page, C. Hettich, B. Aradi, C. Kohler, T. Frauenheim, S. Irle, K. Morokuma, Chem. Sci. 5, 3493 (2014)

O 16.9 Mon 17:15 MA 141

Water splitting reaction on polar Lithium Niobate surfaces — •Christof Dues[1], Wolf Gero Schmidt[2], and Simone Sanna[1] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Department Physik, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn

Water splitting is a highly promising environment friendly approach for hydrogen production. It is often discussed in the context of carbon-dioxide-free combustion and storage of excess electrical energy after conversion to chemical energy. Since the oxidation and reduction reactions are related to significant over-potentials, the search for a suitable catalyst is of particular importance. Ferroelectric materials, e.g. Lithium Niobate (LN), attracted considerable interest in this respect. On the one hand, the spontaneous internal polarization results in enhanced life-times of photo-generated charge carriers. At the other hand, the presence of surfaces with different polarization and chemistry leads to spatial separation of oxidation and reduction reactions. Employing DFT and a simplified thermodynamic approach to calculate Gibbs energy differences, we present an efficient method to estimate the over-potentials related to the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) on both polar $LiNbO_3$(001) surfaces. Our calculations show that the OER and HER over-potentials are lower on the negative (1.27 V) and positive (0.39 V) LN surface, respectively. Calculations within the NEB method reveal the barrier height between the intermediate steps of the OER and HER reactions.

O 16.10 Mon 17:30 MA 141

Tensor-train approximations for catalytic reaction systems — •Patrick Gelss[1], Sebastian Matera[1], and Christof Schütte[1,2] — [1]Freie Universität Berlin, Germany — [2]Zuse Institute Berlin, Germany

For modeling heterogeneous catalytic processes, kinetic Monte Carlo (kMC) simulations have become an important tool since direct molecular dynamics simulations of rare-event systems are prohibitive. However, the drawback of kMC is the large number of simulations needed to capture the relevant dynamics. We present an alternative approach, which mitigates the curse of dimensionality and directly solves a Markovian master equation corresponding to a given microkinetic mechanism by exploiting the tensor-train (TT) format [1]. Different numerical integration methods and step-size adaptation techniques enable a tunable accuracy and linear scaling in the system size for a large range of input parameters. We benchmark the TT approach against highly accurate kMC simulations for catalytic processes based on nearest-neighbor interactions [2], e.g. a model for the CO_2 fixation into methanol at a Cu/ZrO_2 interface [3].

[1] P. Gelß, S. Matera, C. Schütte, J. Comput. Phys., 314, pp. 489-502 (2016)

[2] P. Gelß, S. Klus, S. Matera, C. Schütte, J. Comput. Phys., 341, pp. 140-162 (2017)

[3] Q.-L. Tang, Q.-J. Hong, Z.-P. Liu, J. Catal., 263, pp. 114-122 (2009)

O 16.11 Mon 17:45 MA 141

Enthalpy consistent finite difference lattice Boltzmann method for catalytic flow simulations — •Daniel Berger[1], Ana-Sunčana Smith[2,3], David Smith[3], and Jens Harting[1,4] — [1]Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy — [2]Institute for Theoretical Physics I, University of Erlangen-Nürnberg — [3]Ruđer Bošković Institute, Zagreb, Croatia — [4]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

Many catalyst devices employ porous or foam-like structures to optimize the surface to volume ratio in order to maximize the catalytic efficiency. The porous structure leads to a complex macroscopic mass and heat transport. Local heat accumulation changes the local reaction conditions, which in turn affects the catalytic turn over rate and eventually compromises the stability of the catalytic device.

We present a coupled finite differences thermal lattice Boltzmann model (FD-LBM) to simulate catalytic reactions through porous media. The thermal LBM is used to solve the heat and mass transport in the gas domain, while the chemical surface reactions are incorporated in a very flexible fashion through the flux boundary conditions at the walls. This scheme is further augmented by a finite difference solver to solve the heat equation in the solid and across the gas-solid interface for a consistent treatment of the reaction enthalpy.

To show the strength and flexibility of this model and our implementation, we will report the catalytic turn-over for a wide range of porosities and reaction conditions.

O 16.12 Mon 18:00 MA 141

Atomic and Electronic Structure of Alkali-Doped Zeolites from First Principles — •Debalaya Sarker, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der

MPG, Berlin 14195, Germany

Zeolites posses a crystalline nanoporous aluminosilicate framework with tunable composition, making them ideal candidates for catalytic applications. The substitution of $[\mathrm{SiO_4}]$ tetrahedra by negatively charged $[\mathrm{AlO_4}]^-$ requires inclusion of counterions. In addition, zeolites readily accommodate dopants, in particular alkali metals [1]. The distribution and concentration of dopants and counterions determine solvated electron density distribution and the electrostatic field inside the zeolitic pores, which have a strong influence on sorbed molecules. We study pristine and M-doped MX and MY zeolites (M = Na, K, Cs), using density-functional theory with a semi-local (PBE) and a hybrid (HSE06) functional with an *ab initio* van der Waals correction [2]. For different species of the alkali metals, the positions of the counterions in undoped zeolites are found to vary, contrary to the commonly assumed particular cation sites in FAU-type zeolites [3]. Also, the position of counterions with respect to the six-membered ring is found to correlate with electronegativity of the M atom. We found that the distribution of solvated electrons inside the pores is strongly affected by the dopant type and location.
[1] L. R. M. Martens *et al.*, Nature **315**, 568 (1985)
[2] A. Tkatchenko and M. Scheffler, PRL **102**, 73005 (2009)
[3] D. H. Olson, Zeolites **15**, 439 (1995)

O 17: Solid-liquid interfaces: Reactions and electrochemisty I (joint session O/CPP)

Time: Monday 15:00–16:30 Location: MA 144

O 17.1 Mon 15:00 MA 144

Towards size-selected supported Pd clusters in aqueous environment — •Nicolas Bock, Astrid de Clercq, Clara Rettenmaier, Ueli Heiz, and Friedrich Esch — Chemistry Department & Catalysis Research Center, Technische Universität München, Garching, 85747, Germany

Supported Palladium nanoparticles have been widely investigated as efficient electro- and photo-electro-catalysts. However, for the smaller sub-nanometer Pd clusters, little is known about their size-dependent catalytic properties and stability in aqueous environments. Since this non-scalable size regime bears the potential of high catalytic activity, we aim at finding new ways to prepare and study size-selected Pd clusters via controlled electrochemical decomposition.

To this purpose we have investigated the controlled decomposition of Pd-polyoxo-metalates [1] under specific electrochemical potential and pH conditions, taking advantage of their precise stoichiometry and redox properties. The investigation bases on Electrochemical Scanning Microscopy (ECSTM) and Rotating Disk Electrode (RDE) measurements. Reactivity measurements on single clusters using the STM tip as a microelectrode for hydrogen evolution monitoring are work in progress.

[1] P. Yang, Y. Xiang, Z. Lin, B. S. Bassil, J. Cao, L. Fan, Y. Fan, M.-X. Li, P. Jiménez-Lozano, J. J. Carbó, et al., Angewandte Chemie International Edition 2014, 53, 11974-11978.

O 17.2 Mon 15:15 MA 144

Probing ultrafast processes at electrode-aqueous solution interfaces with laser induced photovoltage measurements — •Yujin Tong, François Lapointe, Martin Wolf, and R. Kramer Campen — Fritz-Haber-Institut, Abt. Physikalische Chemie, 14195 Berlin, Germany

A conventional potentiostat that typically employed for a three electrode electrochemical system has a time resolution of, at best, 1 μ s (bandwidth above 1MHz) [Bard, A.J., Electrochemical methods: fundamentals and applications, New York: Wiley, (1980), Chapter 15]. However, many charge transfer processes happen on pico- to femtosecond time scales. To measure such fast kinetics, all-optical pump probe techniques using ultrafast lasers are usually adopted. In this contribution, we demonstrate that, using a sequence of two ultrashort laser pulses of different photon energies and detection of the laser induced photovoltage by a slow potentiostat as a function of the delay between the two incident pulses, ultrafast charge transfer kinetics on femtosecond timescales can be resolved. For example, we used a UV laser to trigger electron transfer from a gold electrode to $\mathrm{Na_2SO_4}$ aqueous solution and then a second laser in middle or near infrared region was employed to interact with the species that generated by the freshly generated electron. The life time as well as the spectrum of the transient species is consistent with the solvated electron at the interface.

O 17.3 Mon 15:30 MA 144

The Reactivity of Individual 'Defect'-Sites on Electrochemically Roughened Pt(111) — •Leon Jacobse[1], Marcel J. Rost[2], and Marc T.M. Koper[1] — [1]Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands — [2]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands

Platinum is arguably the most stable, highly active electrocatalyst under oxidizing conditions in acidic media. Nonetheless, the poorly understood electrode degradation process strongly limits the economic feasibility of large scale applications.

Previously, we have shown by combination of simultaneous cyclic voltammetry and in-situ EC-STM that the total electrochemical signal of Pt(111) is directly correlated to its surface roughness [1]. This analysis, however, did not yet provide a rationale for this correlation. A detailed analysis of the EC-STM images provides information on the atomic-scale structure of the formed Pt nano-islands and their evolution. Correlating the resulting density of specific surface sites to the different hydrogen adsorption features in the voltammetry, allows us to determine the electrochemical reactivity of formed step and kink sites on the roughened surface. This finally delivers an insight on how to describe the electrochemical reactivity not only of the observed nano-islands but also of Pt nanoparticles in general.
[1] L. Jacobse, Y.-F. Huang, M.T.M. Koper, M.J. Rost, Nature Materials, accepted (2017)

O 17.4 Mon 15:45 MA 144

Correlation of Surface Site Formation to Nano-Island Growth in the Electrochemical Roughening of Pt(111) — Leon Jacobse[1], Yi-Fan Huang[1], Marc Koper[1], and •Marcel Rost[2] — [1]Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands — [2]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands

Platinum plays a central role in a wide variety of electrochemical devices. Electrode degradation, especially under oxidizing conditions, forms an important barrier for the widespread of applications. Although it is known that repeated oxidation and reduction of platinum electrodes results in irreversible surface structure changes, over thirty years of research did not yet yield to a conclusive description of this process on the atomic level; even not for well-defined single crystal surfaces.

Using a special EC-STM, which is capable of measuring the electrochemical signals simultaneously during imaging in operando, we directly correlate, for the first time, the evolution of the hydrogen adsorption peaks on Pt(111) to the observed roughening of the surface. In the later stages, we find a strong correlation between the evolution of the roughness and the absorption peaks clearly indicating that each created step contributes equally strong to the adsorption signal as well as to the roughness. However, and fully surprising, in the early stage step edges are created that seem to be chemically "dead".

O 17.5 Mon 16:00 MA 144

Driving hyrodrogen evolution and oxidation on Pt with femtosecond laser pulses — •Gregor Zwaschka, Yujin Tong, Martin Wolf, and R. Kramer Campen — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The Hydrogen Evolution and Oxidation Reactions (HER/HOR) on Pt have been studied for decades due to their fundamental interest and importance in applications such as electrolyzers and fuel cells. Despite much effort there is no clear view of the mechanism of these reactions that can explain the large dependence of their rates on surface structure, pH and electrolyte. Because the HER/HOR on Pt are fast, one possible explanation for the challenge in obtaining such mechanistic insight is that intermediates exist on the Pt electrode surface at very low concentrations under steady state reactive conditions. In principle such a limit can be overcome by rapidly and transiently increasing the amount of reactants present and characterizing their effect. Here we present our efforts to trigger the HER/HOR on Pt using femtosecond laser pulses. The resulting, laser-induced voltammogram clearly shows that the femtosecond pulse train induces HER/HOR and that the magnitude of this effect depends on crystal face in a manner rationalizable by the surface electronic structure. Control experiments varying pulse lengths, energies and the frequencies of the incident field suggest that we induce the HER/HOR by creating a population of hot electrons. Theses results offer a novel experimental window on the HER/HOR and are a first step in experimentally characterizing the mechanisms of these important reactions.

O 17.6 Mon 16:15 MA 144

On-surface synthesis of covalent architectures for energy conversion chemistry — •Patrick Alexa[1], Doris Grumelli[2], Diana Hötger[1], Vjay Vias[3], Bettina Lotsch[1,4], Rico Gutzler[1], and Klaus Kern[1,5] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Universidad Nacional de La Plata, 1900 La Plata, Argentina — [3]Marquette University, Milwaukee, WI 53233, USA — [4]University of Munich (LMU), 81377 Munich, Germany — [5]Ecole Polytéchnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Creating nanostructures in a bottom-up approach by using molecular precursors allows for the fabrication of tailored nanomaterials for specific applications such as energy conversion. In particular (metal)organic networks synthesized in UHV on crystalline surfaces can be used as efficient electrocatalysts. Inspired by the photocatalytic hydrogen evolution properties of triazine-containing bulk covalent organic frameworks, we investigate structurally similar 2D networks for their propensity for the hydrogen evolution reaction. In this work we synthesize two-dimensional covalent polymers from 2,4,6-tri-(4-bromophenyl)-1,3,5-triazine on Au(111) and visualize their topography by scanning tunneling microscopy. The polymer-decorated surface shows a promising improvement for the hydrogen evolution reaction compared to bare Au(111) in electrocatalytic experiments. The influence of electrolyte exposure and electrocatalytic conditions on the polymer structure is discussed. These results highlight the capability of single-layer functional 2D polymers for electrocatalysis.

O 18: Focus Session: Frontiers in Reducible Oxide Surface Science II

Time: Monday 15:00–18:15 Location: HE 101

Invited Talk O 18.1 Mon 15:00 HE 101

Surface chemistry of ruthenates — •Ulrike Diebold[1], Daniel Halwidl[1], Wernfried Mayer-Schmözer[1,2], Martin Setvin[1], Florian Mittendorfer[1,2], Josef Redinger[1,2], and Michael Schmid[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Center for Computational Materials Science, TU Wien, Vienna, Austria

Ternary oxides with a perovskite-type crystal structure are of increasing interest in energy-related applications such as solid oxide fuel/electrolysis cells and (photo-) electrocatalysis. Surface science studies can provide an atomic-scale understanding of relevant fundamental processes, but appropriate model systems with a well-defined surface structure are rare. Here we report our results on the cleaved CaO and SrO-terminated surfaces of the Ruddlesden-Popper materials $Ca_3Ru_2O_7$ and $Sr_3Ru_2O_7$. Surfaces can easily be prepared by exfoliation in UHV, which provides large, defect-free terraces that are ideal for atomic-scale investigations. We used STM and nc-AFM in combination with XPS and DFT to investigate the adsorption of H_2O [1,2] and O_2. We find that results on the related binary oxides give a good first guide for the adsorption behaviour, and that the tilting and rotation of the materials' octahedra strongly influence the ordering of overlayers. [1] D. Halwidl, et al. Nature Mater. 15 (2016) 450. [2] D. Halwidl, et al., Nature Comm. 8 (2017) 23.

Invited Talk O 18.2 Mon 15:30 HE 101

Multiscale modelling of metal oxide interfaces and nanoparticles — •Kersti Hermansson — Department of Chemistry-Ångström Laboratory, Uppsala University, Uppsala (Sweden)

In the scientific literature, a full arsenal of experimental methods are being used to help characterize redox-active metal oxide surfaces and interfaces such interfaces. At the same time, the number of theoretical studies steadily increases, providing mechanistic information at a detail that is hard to beat by experiment. Here the major challenges are (i) how to build a structural model that captures the complexity and imperfections of the real system at hand, and (ii) how to find interaction models that are good enough.

I will discuss some efforts in the development of multiscale modelling approaches for surfaces and interfaces of metal oxides (e.g. CeO2, ZnO, MgO) with and without interacting molecules (e.g. water), including combinations of DFT, tight-binding-DFT, and reactive force-field simulations. Can calculations without explicit electrons really be used instead of quantum-mechanical calculations when the electrons are so closely coupled to the functionality as they are for redox-active metal oxides?

I will also inform about the European Materials Modelling Council (https://emmc.info/), and our efforts to promote the use of materials modelling in industry and the quality of the modelling results; the EMMC is open to everyone interested.

O 18.3 Mon 16:00 HE 101

MnO(001) thin films on Au(111) — •Christoph Möller and Niklas Nilius — Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany

A variety of oxidation states and a high reactivity make manganese oxide a promising material for applications in heterogeneous catalysis. Using STM and XPS, we have probed the structural and electronic properties of ultrathin MnO films deposited on the Au(111) surface. At low coverage, the oxide crystallizes into regular islands with up to 50 nm diameter. Their surface exposes either a 2x2 reconstruction or various stripe phases, depending on the island height. The MnO band gap was determined to 2.8 eV, while the first field-emission resonance occurs at 3 eV, indicating a drastic decrease of the gold work function upon MnO deposition. With increasing thickness, the oxide grows into a polycrystalline, non-conductive film, whose stoichiometry increasingly deviates from MnO.

O 18.4 Mon 16:15 HE 101

Electrochemical Characterization of Reducible Oxide Surfaces — •Ladislav Kavan — J. Heyrovsky Institute of Physical Chemistry, Dolejskova 3, 182 23 Prague, Czech Republic

The electronic band structure of semiconducting oxides (TiO2 or SnO2) is relevant to photo/electrochemistry and energy applications. The position of conduction band (CB) edge controls reductive photocatalytic reactions (e.g. hydrogen formation from water or CO2-reduction to solar fuels), Li-insertion electrochemistry, recombination blocking in perovskite solar cell and open-circuit potential of dye-sensitized solar cell. Recently, the reduction of CO2 to methane attracted attention for investigation of Mars atmosphere. The ALD-grown TiO2 and SnO2 layers are useful for electron selective contacts in perovskite solar cells. However, there is a considerable controversy about the position of CB in TiO2 (anatase, rutile, including the crystals with distinguished facets). The conflict is rationalized by considering the adsorption of OH- and H+ ions from the electrolyte solution on the electrode surface [5]. The facet specific electrochemistry of water splitting on TiO2 is addressing both the CB position and the electrocatalytic activity of the relevant crystal face. Doping of SnO2 by F- or Sb5+ provides the quasi-metallic (degenerate semiconductor) material, but little is known about similar doping-induced behavior of TiO2. We have recently found purely metal-like electrochemical properties of Ta-doped, optically transparent thin films of TiO2 (anatase) made by pulsed-laser deposition.

15 min. break

O 18.5 Mon 16:45 HE 101

Mixed nano-oxides: microscopic mechanisms behind their structural and electronic characteristics — •Claudine Noguera, Jacek Goniakowski, and Ha-Linh T. Le — Institut des Nanosciences de Paris CNRS and Université Pierre et Marie Curie, Paris, France

Doped and especially mixed (ternary) oxides represent promising materials with many potential applications in spintronics, materials for energy and environment, etc. Indeed, combining two cations of different size and/or electronegativity is expected to allow modulating the structural and electronic properties of the resulting alloy. However, there are presently large gaps in our understanding of the formation and properties of such mixed-oxides, especially at the nanoscale.

In this context, considering the technological importance of titanium and other transition metal oxides, we have focused on mixed transition metal oxides of XYO3 stoichiometry, within two architectures displaying low dimensional effects. Relying on first principles simulations, we analyze and compare the electronic properties of Ti2O3/X2O3 heterostructures and TiXO3 honeycomb monolayers deposited on an Au(111) substrate (X=V, Cr, Fe) and we highlight the driving forces toward mixing.

O 18.6 Mon 17:00 HE 101

Improving Adhesion at weakly-interacting metal/oxide interfaces — Ha-Linh T. Le[1], •Jacek Goniakowski[1], Claudine Noguera[1], Alexey Koltsov[2], and Jean-Michel Mataigne[2] — [1]Institut des Nanosciences de Paris, CNRS, 75005 Paris — [2]ArcelorMittal Maizières Research, 57280, Maizières lès Metz

The control of adhesion at metal/oxide interfaces is of a key importance for a large variety of applications, involving either 2D or 3D metal deposits on oxide substrates. More recently it has also been addressed in the context of anti-corrosive zinc coating of advanced high strength steels. Indeed, selective oxidation and surface segregation of strengthening elements, such as Al, may lead to a formation of an oxide film on the steel surface which dramatically reduces zinc adhesion.

In this context, we report a thorough ab initio and Monte Carlo study of adhesion at a zinc/alpha-alumina(0001) interface. We find that the interaction of zinc with bare non-polar terminations of alumina is indeed weak but that it can be improved by either surface pre-hydroxylation or by metallic buffers. While the performance of single-component buffers may degrade upon oxidation, that of realistic multi-component ones (e.g. stainless steel) remain satisfactory under a large span of oxidizing conditions due to the separation of metal and oxide components in the buffer and the suppression of the weak oxide/zinc and moderately strong alumina/metal interfaces. More generally, thanks to the possibility of selective oxidation and component segregation, multi-component buffers appear as promising solutions for improving adhesion at weakly interacting metal/oxide interfaces.

O 18.7 Mon 17:15 HE 101

A DFT study of the (011) and (110) surfaces of rutile VO$_2$ — •Florian Mittendorfer[1,2], Jakub Planer[1,2], Wernfried Mayr-Schmölzer[1,2], and Josef Redinger[1,2] — [1]Center for Computational Materials Science, TU Wien, Vienna, Austria — [2]Institute of Applied Physics, TU Wien, Vienna, Austria

Vanadium dioxide is a promising material with potential applications for fast electronic or optical switching. These applications are related to a structural and electronic transition from monoclinic to a rutile phase at 340K. Our results show that standard DFT (PBE) approaches give a reasonable description of the metallic rutile phase, while more advanced approaches, such as meta-GGA+U (SCAN) or hybrid functionals are needed to obtain the correct band gap of ∼0.7 eV for the monoclinic phase. In addition, I will discuss the stability of various terminations for the rutile VO$_2$(011) and (110) surface and compare them to recent experimental STM data.

O 18.8 Mon 17:30 HE 101

identification of active sites for water oxidation with extremely low overpotential on multicomponent spinel Co$_x$Ni$_{1-x}$Fe$_2$O$_4$**(001) surfaces** — •hamidreza hajiyani and rossitza pentcheva — Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen

Using density functional theory calculations with an on-site Hubbard term (DFT+U) we explore the effect of cation substitution and surface termination on the performance of Co$_x$Ni$_{1-x}$Fe$_2$O$_4$(001) as an anode material in the oxygen evolution reaction (OER). To identify the active sites, we investigated the performance of different reaction sites (Fe, Co, Ni and O) at the B-layer with 5-fold coordinated Co/Ni and with an additional 0.5 ML Fe at the (001) spinel surface. Our results indicate that mixing of Co and Ni in equal concentrations (x=0.5) lowers the overpotential over the end members for the majority of reaction sites. Comparison of the overpotentials indicates that surface Co cations on the 0.5 ML Fe termination are the most active sites with the lowest theoretically reported overpotential of 0.30 V. We have shown that this beneficial performance correlates with the modification of the binding energies of intermediate species to the surface. Analysis of the electronic properties and spin densities indicate that the oxidation state of Fe changes from +3 in the bulk to +2 on the 0.5 ML Fe surface, while Co and Ni cations at this termination preserve the bulk oxidation states of +2. Funding by the DFG within SPP1613 is gratefully acknowledged.

O 18.9 Mon 17:45 HE 101

Activation of O$_2$ adsorbed on (Ca,Sr)$_3$Ru$_2$O$_7$ surfaces: a DFT study — •Wernfried Mayr-Schmölzer[1,2], Daniel Halwidl[2], Florian Mittendorfer[1,2], Ulrike Diebold[2], Josef Redinger[1,2], and Michael Schmid[2] — [1]Center for Computational Materials Science, TU Wien, Vienna, Austria — [2]Institute of Applied Physics, TU Wien, Vienna, Austria

Transition metal perovskite oxides are promising materials for a wide range of applications as diverse as fuel cells and catalysts. Surprisingly not much work has been done on their surface properties regarding oxygen transport and redox properties. Recently the adsorption of O$_2$ as a charged molecule has been predicted by DFT on defective SrTiO$_3$[1], and La$_2$NiO$_4$[2] surfaces. Here, we present a theoretical analysis including many-electron methods of O$_2$ adsorption on defect-free rocksalt-like SrO and CaO surfaces of Ruddelsden-Popper type Sr$_3$Ru$_2$O$_7$(001) and Ca$_3$Ru$_2$O$_7$(001). We observe the adsorption of molecular O$_2$ as a charged superoxo species on both defect-free materials. The DFT adsorption energies are high, up to 1.4 eV on both oxides, which we attribute to the overestimation of the electron affinity of O$_2$ by standard semi-local functionals, making the charging of the O$_2$ adsorbate too easy. Using beyond-DFT methods such as hybrid (HSE) functionals and advanced many-electron methods (RPA, G$_0$W$_0$) to properly describe the adsorption properties, we calculate an RPA adsorption energy of 0.72 eV in very good agreement with experimental values.

[1] Staykov, A., Chemistry of Materials, 27(24), 8273-8281.
[2] Akbay, T., J. Mater. Chem. A, 4(34), 13113-13124.

O 18.10 Mon 18:00 HE 101

In-situ studies of the reduction of ultrathin BaTiO$_3$ on Pt(111) — •Jonas Pantzer[1], Stefan Förster[1], Jan Ingo Flege[2], Jens Falta[2], and Wolf Widdra[1,3] — [1]Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Universität Bremen, 28359 Bremen, Germany — [3]Max-Planck-Institute for Microstructure Physics, 06120 Halle, Germany

Reduced ultrathin films derived from the prototypical perovskite oxides BaTiO$_3$ and SrTiO$_3$ have recently attracted attention due to the their transformation into two-dimensional oxide quasicrystals (OQCs) on a hexagonal metal support [1]. For BaTiO$_x$ on Pt(111), the OQC formation proceeds in two steps via an amorphous two-dimensional wetting layer[2].

Here we report on in-situ low energy electron microscopy (LEEM) studies of morphological changes starting from stoichiometric BaTiO$_3$(111) islands on Pt(111). At 1350 K the genesis and movement of a diffusion front of an amorphous two-dimensional wetting layer on the bare platinum is observed, which starts at the BaTiO$_3$(111)-islands. Subsequently, a second, much slower, diffusion front is observed at the edges of the BaTiO$_3$(111)-islands, indicating a crystallisation of the wetting layer into differently oriented BaTiO$_3$(111).

[1] Förster et al., Nature 502, 215 (2013)
[2] Förster et al. Ann. Phys. 529, 1600250 (2017)

O 19: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Monday 15:00–17:15 Location: HL 001

O 19.1 Mon 15:00 HL 001

Non-adiabatic Dynamics in Single-Electron Tunneling Devices with Time-Dependent Density Functional Theory — •Niklas Dittmann[1,2,3], Janine Splettstoesser[2], and Nicole Helbig[3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [2]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Gothenburg, Sweden — [3]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

The recent advance of various single-electron sources in solid-state setups has sparked interest in the investigation of electronic transport at the single-particle level. In our recent work (N. Dittmann, J. Splettstoesser, N. Helbig, arxiv:1706.04547), we put forward time-dependent density-functional theory to calculate the dynamics of interacting electrons in single-electron tunneling devices. As a physical system, we analyze a single-electron source which is built by a quantum dot tunnel-coupled to a nearby electron reservoir and driven by a time-dependent gate voltage. By using analogies with quantum-transport theory, we extract a time-nonlocal exchange-correlation potential for a Hubbard U on-site interaction on the quantum dot. The time nonlocality manifests itself in a dynamical potential step, which we explicitly link to physical relaxation time scales of the electron dynamics. Finally, we discuss prospects for simulations of larger mesoscopic systems.

O 19.2 Mon 15:15 HL 001

Dissipative exchange-correlation functional in QED-TDDFT — •Camilla Pellegrini[1], Ilya Tokatly[2,3], and Angel Rubio[2,4] — [1]Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain — [3]IKERBASQUE, Basque Foundation for Science, 48001 Bilbao, Spain — [4]Max Planck Institute for the Structure and the Dynamics of Matter, Luruper Chausse 149, 22761 Hamburg, Germany

Time-dependent density functional theory has been recently extended to treat many-electron systems coupled to quantized electromagnetic modes. Here we discuss the implications of this approach for the theory of open quantum systems. In particular we show that in the limit of continuous spectrum of photon modes, QED-TDDFT naturally leads to time-dependent density functional theory for dissipative systems coupled to the Caldeira-Leggett bath. We consider the application to the Ohmic spin boson model and show that the developed approximation to the exchange-correlation functional describes the natural linewidth of the electronic linear density response function.

O 19.3 Mon 15:30 HL 001

Electric and magnetic response properties of solids from the current density — •Rubén Rodríguez Ferradás[1], Pina Romaniello[2], and Arjan Berger[1] — [1]LCPQ, University of Toulouse, France — [2]LPT, University of Toulouse, France

The evaluation of the macroscopic polarization and magnetization of solids is problematic when periodic boundary conditions are used because surface effects are artificially removed. This poses a problem unless surface effects can be reformulated in terms of bulk quantities [1-5]. In this work we show the advantage of calculating electric and magnetic response properties of solids using the current density as basic variable. An efficient approach to calculate the current density is time-dependent current-density-functional theory. We will show results for optical properties of solids using a recently developed functional [6]. We will also discuss how the magnetization can be described within this framework.

[1] F. Kootstra, P.L. de Boeij, and J.G. Snijders, J. Chem. Phys. 112, 6517.

[2] J.A. Berger, P.L. de Boeij, and R. van Leeuwen, Phys. Rev. B 71, 155104 (2005).

[3] P. Romaniello and P.L. de Boeij, Phys. Rev. B 71, 155108 (2005).

[4] J.A. Berger, P. Romaniello, R. van Leeuwen, and P.L. de Boeij, Phys. Rev. B 74, 245117 (2006).

[5] J.A. Berger, P.L. de Boeij, and R. van Leeuwen, Phys. Rev. B 75, 035116 (2007).

[6] J.A. Berger, Phys. Rev. Lett. 115, 137402 (2015)

O 19.4 Mon 15:45 HL 001

Coupling Maxwell's equations to the time-dependent Kohn-Sham equations: near-field effects and electromagnetic backreaction — •Rene Jestaedt[1], Micael Oliveira[1], Angel Rubio[1,2,3], and Heiko Appel[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, USA — [3]Nano-bio Spectroscopy Group and ETSF, Universidad del País Vasco, 20018 San Sebastián, Spain

Induced currents in large molecular and condensed matter systems are non-negligible and can affect the conductivity and the optical properties of the system. In the present work, we have implemented the real-time propagation of Maxwell's equations in Riemann-Silberstein representation to use standard unitary propagation techniques in the TDDFT code octopus [1]. The Maxwell and the Kohn-Sham system are coupled via a predictor-corrector method to obtain a self-consistent time-evolution of the total system [2]. Explicitely solving the microscopic Maxwell's equations also allows us to determine the optical properties of the system directly from the Maxwell fields. We show near-field effects of a full Maxwell-matter and matter-Maxwell coupling for plasmon excitations in metallic nanoparticles [2,3] and for ring-currents in organic molecules [2].

[1] Alejandro Varas et al., J. Phys. Chem. Lett. 2015, **6**, 1891-1898 / [2] R. Jestädt et al., (to be submitted) / [3] X. Andrade et al., Physi. Chemistry Chem. Physics 2015, **17** 31371-31396

O 19.5 Mon 16:00 HL 001

Enhancing excitation energy and charge transfer with strongly correlated light-matter interaction — •Christian Schäfer[1], Michael Ruggenthaler[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

Förster excitation energy and charge transfer are fundamental processes of chemical reactions and connected to interesting quantities such as correlation. Often this correlation is taken as fixed property of the system.

In the current work, we present how the coupling to cavity photons in a minimal realistic molecular system can drastically alter transfer characteristics, e.g. renders the excitation transfer to be distance independent [1,2]. The photonic interaction can imprint fermionic correlation on arbitrary distances.

The exact real-space description is suited to describe transfer and correlation in a unprejudiced ab-initio picture and allows us to extend our insights beyond common quantum-optical approximations.

[1] X. Zhong et al., Angew Chem Int Ed Engl. **56(31)**, 9034 (2017).
[2] M. Slootsky et al., PRL **112**, 076401 (2014).

O 19.6 Mon 16:15 HL 001

Effects of electronic correlations on the magnetic properties of organometallic molecules — •Sumanta Bhandary and Silke Biermann — Centre de Physique Thèorique, Ecole Polytechnique, 91128 Palaiseau, France

The realm of molecular spintronics relies on the external accessibility of molecular magnetic states. In correlated organometallic complexes, a delicate balance between the crystal field, Coulomb repulsion and dynamical hybridization between metal center and organic ligands dictates the electronic and magnetic properties and often poses challenges for an accurate theoretical modelling. We have employed density functional theory (DFT), the GW approach and Anderson's impurity model (AIM) technique to study the ground state electronic and magnetic properties of transition metal-based porphyrin and phthalocyanine molecules, both in the gas phase [1] as well as while adsorbed on surfaces. Our study reveals that the dynamical correlation effects are important in order to accurately estimate spin-transition energies, magnetic anisotropy energies as well as the ground state electronic configurations in the molecular complexes. We have explored the manipulation of surface molecule interactions to externally influence the electronic and magnetic properties of the molecular system.

[1] S. Bhandary, M. Schüler, P. Thunström, I. di Marco, B. Brena, O. Eriksson, T. Wehling, and B. Sanyal, Phys. Rev. B **93**, 155158 (2016).

O 19.7 Mon 16:30 HL 001

Structural, electronic and optical properties of cubic and tetragonal $SrTiO_3$: a DFT study including many-body effects — •Vijaya Begum, Markus E. Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg.

$SrTiO_3$ (STO) is of fundamental interest as a substrate material in oxide electronics. The bulk undergoes a phase transition from the cubic to a tetragonal structure at T=105 K accompanied by characteristic antiferrodistortive rotations of the TiO_6 octahedra. We present a systematic comparison of the performance of the gradient corrected exchange correlation functional (GGA), the strongly constrained and appropriately normed (SCAN) meta-GGA and the hybrid functional HSE06 with respect to the electronic, structural and optical properties of cubic and tetragonal STO. For the tetragonal structure, SCAN gives a significantly improved description of the structural properties, comparable to HSE06, at a computational cost similar to GGA. The experimental band gap can be reproduced within SCAN with an on-site Hubbard term ($+U$), whereas within GGA the gap is underestimated even for very high U values. We calculate the optical spectrum for both phases, including many-body effects and excitonic corrections within the GW+Bethe-Salpeter equation approach, and compare this to previous theoretical results for the cubic phase [PRB 87, 235102 (2013)] and experiment [PRB 93, 075204 (2016)]. Funding by the DFG within SFB1242, project C02 is gratefully acknowledged.

O 19.8 Mon 16:45 HL 001

Unveiling the mysterious magnetic state of superconducting iron under pressure — •Matteo d'Astuto — Institut NEEL CNRS/UGA UPR2940 25 rue des Martyrs BP 166 38042 Grenoble cedex 9 FRANCE — IMPMC, UMR CNRS 7590, Sorbonne Universités-UPMC University Paris 06, MNHN, IRD, 4 Place Jussieu, F-75005 Paris, France

Compressed iron undergoes a transition from bcc to hcp crystal structure with a loss of ferromagnetism. The magnetic state of the hcp phase has been debated for many decades and experiments give seemingly contradictory results. Mössbauer measurements find no magnetism, however x-ray emission spectroscopy finds remnant magnetism and Raman mode splitting suggests symmetry breaking due to antiferromagnetism. These paradoxical results are consistent with either a paramagnetic state with spin fluctuations faster than Mössbauer timescales or an antiferromagnetic state, afmII, which is undetectable with Mössbauer spectroscopy. We performed neutron powder diffraction measurements in the hcp phase and do not observe afmII order down to 1.8 K, while confirming the existence of a local magnetic moment in the hcp phase with x-ray emission spectroscopy and find it is intrinsic to this phase (1). This local magnetic moment disappears at 30–40 GPa, exactly the same pressure region where superconductivity disappears.

(1) B. W. Lebert, T. Gorni J.-P. Rueff, S. Klotz, M. Casula, A. Juhin, J. M. Ablett, F. Baudelet, T. Straessle, T. Hansen, A. Polian, P. Munsch, G. Le Marchand, Z. Zhang, M. d'Astuto, article in preparation.

O 19.9 Mon 17:00 HL 001

Frist-principle and experimental characterisation of the electronic properties of CaGaSiN3 and CaAlSiN3: impact of chemical disorder — •Jan Minar[1], Ondrej Sipr[2], Robin Niklaus[3], Jonas Hausler[3], and Wolfgang Scgnick[3] — [1]New Technologies Research Center, University of West Bohemia, Pilsen, Czech Rep., — [2]FZU, Academy of Sciences, Czech Rep — [3]Department of Chemistry, University of Munich, Munich, Germany

We report a detailed investigation of the electronic, mechanical and optical properties of the recently discovered nitridogallosilicate CaGaSiN3 which has potential as a LED-phosphor host material. We focus on chemical disorder effects, originating from the Ga/Si site, and compared them to those of isostructural CaAlSiN3. We calculate the elastic moduli and the Debye temperature in terms of quasi harmonical approximation. Spectral properties like the joint density of states (JDOS) are evaluated and the absorption, reflectance and energy loss function are obtained from the dielectric function. The optical band gap of CaGaSiN3 from experiment is compared to the electronic band gap in terms of electronic DOS and band structure calculations. All properties are evaluated for different ordering models of Ga/Si while the experimentally observed substitutional disorder is accounted for by utilizing the Coherent Potential Approximation (CPA). We conclude a shrinking of the band gap for both CaGaSiN3 and CaAlSiN3 due to atomic disorder, which is unfavorable for potential phosphor applications [1]. R. Niklaus, J. Minar, J Häusler, W. Schnick, Physical Chemistry Chemical Physics 19 (13), 9292 (2017)

O 20: Graphen: Adsorption, intercalation and doping II (joint session O/TT)

Time: Monday 16:45–18:15 Location: MA 043

O 20.1 Mon 16:45 MA 043

Initial investigation of the coexistence of different structural conformations, obtained via high temperature deposition of PbPc on epitaxial graphene grown on 6H-SiC(0001) — •Chitran Ghosal[1,2], Samir Mammadov[1], Martina Wanke[1], Florian Speck[1], Thomas Seyller[1], and Christoph Tegenkamp[2] — [1]Professorship of Technical Physics, Institute of Physics, TU-Chemnitz — [2]Professorship of Solid Surfaces Analysis, Institute of Physics, TU-Chemnitz

Epitaxial deposition is one of the well documented ways of doping of graphene[1]. Therefore, it is crucial to be able to study the different possible structural configurations that can be obtained via the deposition techniques.

This study deals with the analysis of different periodic structures obtained via the deposition of PbPc on epitaxial graphene, which was grown on 6H-SiC(0001) surfaces. The graphene was characterized by LEED and high resolution XPS measurements as well as STM. PbPc molecules were deposited afterwards at high temperatures of around 330degC and densely packed molecular films were grown under UHV conditions. Fourier analysis of large scale STM images revealed the coexistence of two non-orthogonal lattice structures (1.2nm X 1.6nm) and (1.35nm X 1.4nm) forming different islands separated by grain boundaries in between. The variability of the structures underlines the weak interaction of the PbPc molecules with the substrate.

[1] I. Gierz, C. Riedl, U. Starke, C. R. Ast, and K. Kern, Nano Lett. 8, 4603 (2008).

O 20.2 Mon 17:00 MA 043

Investigation of PbPc self-assembly on graphene: Atomic resolution and spectroscopy data — •Nhung Nguyen[1,2], Ha Nguyen[1], and Christoph Tegenkamp[1] — [1]TU Chemnitz — [2]Duy Tan University, Vietnam

Shuttlecock-like lead-Phthalocyanine (PbPc) with its two equivalent stable up- and down states corresponding to ON/OFF switch is used for high density data storage of three- orders-magnitude capability higher than the present high density storage materials capability [1]. In addition, absorption of organic molecules on graphene surface due to the charge transfer mechanism between them is one of the promising methods to break the symmetries in graphene, localize the electronic states toward open a bandgap, which makes graphene useful as a nanoelectronics material [2]. Here the self-assembly of PbPc on one monolayer graphene/SiC surface is investigated by means of scanning tunneling microscopy and spectroscopy (STM/STS) in ultra-high vacuum. Due to the weak molecule-substrate interaction as well as the thermodynamic stability, shuttlecock PbPc molecules are only deposited with Pb atom pointing upward (face-up) into the first monolayer, but face-up or face-down states appear randomly on the second layer. The occupied and unoccupied orbitals of PbPc on graphene are distinguished intuitively. The influences of surface coverage, substrate temperature and substrate properties (buffer layer and quasi-free-standing graphene substrates) on self-assembly of PbPc will be discussed. [1] Phys Chem Chem Phys., 2015, 17,23651. [2] PhysRevB., 2009, 80, 033404.

O 20.3 Mon 17:15 MA 043

Physical adsorption on graphene: from ultra-long ranged attraction to full screening of weakly interacting substrates — •Alberto Ambrosetti and Pier Luigi Silvestrelli — via Marzolo 8, 35131 Padova, Italy

The Lifshitz-Zaremba-Kohn (LZK) theory is commonly regarded as the correct large-distance limit for the van der Waals (vdW) interactions between adsorbates and solid substrates. However, recent experiments are challenging the universality of the LZK theory over a broad spectrum of nanoscale materials. By overcoming the conventional *local* permittivity approximation, here we demonstrate that physical adsorption on graphene and other low-dimensional materials can exhibit highly non-trivial features. Substrate-adsorbate vdW interactions can be extremely long-ranged and externally tunable. Moreover, graphene can effectively screen weakly interacting supporting substrates, emerging as an effective tool for the experimental modulation of adsorption processes.

O 20.4 Mon 17:30 MA 043

Advances in ultra-low energy ion implantation of low dimensional materials — •Hans Hofsäss and Manuel Auge — II. Physikalisches Institut, Universität Göttingen, Germany

Doping of 2D materials by ion implantation has unique requirements regarding ion energy, ion energy spread, ion beam optics, sample preparation and sample electrical conductivity. Efficient incorporation of low energy ions into 2D lattices requires energies well below 50 eV. We use a 30 keV mass selected ion beam, guided through differential pumping stages and homogenized by a beam sweep. The beam is then decelerated in a UHV-chamber down to energies as low as 10 eV onto an area of 1 cm^2 up to 2.5 cm^2. Up to now ion sources are available for B, C, N ,F, P, S, Mn, Se, W and Au ions. Ion sources for elements Al, Fe, As and rare earth elements are under development. The implanted areal concentration and elemental composition are verified with in-situ Auger spectroscopy and more quantitative with Rutherford backscattering by implanting into amorphous carbon films as test samples. The detection limit is below 1*10^{14} ions/cm^2 for heavier elements. Implanted B can be analyzed with the ^{11}B(p,2α)α nuclear reaction with a detection limit of about 1*10^{14} B/cm^2. Challenges for ULE ion implantation such as non-flat substrates, charging of substrates, cleaning of surfaces and lateral controlled implantation will be briefly discussed. Some examples for doped graphene and MoS$_2$ are presented

O 20.5 Mon 17:45 MA 043

growth of fe3o4 nanorod arrays on graphene sheets for application in electromagnetic absorption fields — •huanming zhang^1, min zhou^1, yang xu^1, shipu xu^1, yujin chen^2, and yong lei^1 — ^{1}Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693 Ilmenau, Germany — ^{2}Key Laboratory of In-Fiber Integrated Optics, Ministry of Education, College of Science, Harbin Engineering University, 150001 Harbin, China

A facial strategy is developed to fabricate a three-dimensional (3D) Fe3O4 nanorod array/graphene architecture, in which Fe3O4 nanorods with a length and diameter of about 600 and 100 nm, respectively, are grown on both surfaces of the graphene sheets. The measured electromagnetic parameters show that the 3D architecture exhibits excellent electromagnetic wave-absorption properties, that is, more than 99*% of electromagnetic wave energy can be attenuated by the 3D architecture if it is added in only 20 wt*% of the paraffin matrix, as the thickness of the absorber is in the range from 2.38 to 5.00 mm. The analysis of the electromagnetic (EM) absorption mechanism reveals that the excellent EM absorption properties are related to the special 3D architecture, and therefore, the construction of graphene-based 3D heteronanostructures is effective in obtaining lightweight EM absorbers with strong absorption properties.

O 20.6 Mon 18:00 MA 043

Continuous in-plane graphene-hexagonal boron nitride layer from a single molecular precursor — •Federica Bondino^1, Silvia Nappini^1, Igor Píš^{1,2}, Tevfik Onur Menteş^2, Alessandro Sala^2, Andrea Locatelli^2, Stefano Agnoli^3, Mattia Cattelan^3, and Elena Magnano^1 — ^{1}IOM-CNR, Laboratorio TASC, S.S. 14-km 163.5, 34149 Basovizza, Trieste, Italy — ^{2}Elettra - Sincrotrone Trieste S.C.p.A., S.S. 14-km 163.5, 34149 Basovizza, Trieste, Italy — ^{3}Department of Chemical Sciences, University of Padua, Padova 35131, Italy

We will show that it is possible to grow a continuous sp2 hybridized material composed by graphene and hexagonal-boron nitride (h-BNG) in the same two dimensional sheet with the thermal decomposition of a single molecular precursor [1,2]. This surface-synthesis route allows an easy and controlled preparation of an high-quality h-BNG monolayer on the surface of several substrates. The temperature is the principal parameter to selectively grow the h-BNG layer in competition with hybridized B-C-N layers. The reactivity and the confinement of metal nanostructures in the interface between h-BNG and its solid substrate will be discussed in comparison with graphene. Basic processes, chemical composition, substrate interaction and changes accompanying the growth and intercalation process will be discussed based on results obtained by synchrotron radiation experimental techniques, such as high-resolution X-ray photoelectron spectroscopy and microscopy and X-ray absorption spectroscopy. 1. S. Nappini et al. Adv.Funct.Mater. 26, 1120 (2016). 2. S. Nappini et al. Carbon 120, 185 (2017).

O 21: Solid-liquid interfaces: Reactions and electrochemisty II (joint session O/CPP)

Time: Monday 16:45–18:15 Location: MA 144

O 21.1 Mon 16:45 MA 144

Pt modified Ru(0001) electrodes: structure-activity relationship for the CO and MeOH electrooxidation — •Albert K. Engstfeld, Jens Klein, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Bimetallic PtRu catalysts are the most prominent catalyst material in polymer electrolyte membrane fuel cells for the electrooxidation of methanol (MeOH) since it enables the oxidation of the strong binding reaction intermediate CO from the surface at much lower overpotentials compared to a bare Pt catalyst. The underlying process is attributed to a so-called Langmuir Hinshelwood bifunctional mechanism, where the CO oxidation from Pt and Ru sites is promoted by the preferential adsorption of oxygen on neighboring Ru sites. In this work, we will show in comparison the electrocatalytic CO and MeOH oxidation on well defined Pt-modified Ru(0001) electrodes (surface alloys and Pt sub-/multilayer structures), prepared under UHV conditions and characterized on an atomic scale level with scanning tunneling microscopy (STM). For the surface alloys as well as submonolayer Pt-modified Ru(0001) we will show that the formation of bifunctional sites is indeed beneficial for the CO electrooxidation but is surprisingly inactive for the MeOH electrooxidation. On Pt multilayer structures, thus a surface without bifunctional sites, the MeOH electrooxidation is significantly more active compared to the mixed surfaces. Based on these results we will discuss the rate-limiting steps for the MeOH electrooxidation on these surfaces and discuss the influence of related electronic and geometric effects on both the CO and MeOH oxidation.

O 21.2 Mon 17:00 MA 144

Influence of Pt step sites on the electro-oxidation of CO — •Jens Klein, Valeria Chesnyak, Evelyn Artmann, Julian Bösking, Albert K. Engstfeld, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm

The performance of the CO electro-oxidation on Platinum (Pt) catalysts strongly depends on the surface structure of the catalyst. It has been reported that Pt electrodes with a large number of low coordinated step sites show an enhanced activity for the electro-oxidation of an adsorbed monolayer of CO, which was ascribed to active sites on the step edges.[1]

In this work we investigated the role of Pt steps in the electro-oxidation of CO on Pt electrodes under continuous CO supply (bulk CO oxidation). We prepared Pt(111) single crystal electrodes and varied the Pt step edge density by physical vapor deposition of Pt on the crystal under UHV conditions. The structural properties were characterized by scanning tunneling microscopy (STM). To identify the actual role of Pt step edges we blocked the respective sites, by decorating the Pt steps with a narrow Au film, since Au supported on Pt(111) was reported to be inert for the CO oxidation.[2] The electrocatalytic measurements, which were performed in an electrochemical flow cell, provide information on the role of the Pt steps in the CO oxidation and consequences of these findings will be discussed.

[1] G. García et al., ChemPhysChem. 12 (2011) 2064.

[2] D. C. Skelton et al., J. Phys. Chem. B, 103 (1999) 964.

O 21.3 Mon 17:15 MA 144

Comparing solvation effects on adsorbates at water/Pt(111) interface with implicit and explicit solvents — •Sung Sakong and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

For a realistic description of the elementary electrocatalytic processes at electrode/electrolyte interfaces, an adequate method to treat the solvated molecules at the interface is necessary. Since the solvation in liquid solvent requires thermodynamic sampling which is computationally demanding within ab initio molecular dynamics (AIMD) approach, numerically efficient implicit solvent methods which address solvation effects through a polarization potential and a corresponding electrostatic energy are becoming increasingly popular.

The structure of liquid water in the bulk and near electrode surfaces differs. Therefore we consider an implicit solvent method that determines cavitation on the fly using the charge density evaluated by quantum chemical methods. We will compare solvated reaction intermediates in the methanol electro-oxidation at the Pt(111)/water interface using an implicit solvent method and using explicit solvating water layer at the interface in order to assess the reliability of the implicit solvent approach.

[1] J. Chem. Phys. **142**, 234107 (2015).

[2] ACS Catal. **6**, 5575 (2016).

[3] Electrocatalysis **8**, 577 (2017).

O 21.4 Mon 17:30 MA 144

Microcalorimetric measurement of double layer charging in ionic liquids — •Jeannette Lindner[1], Fabian Weick[1], Stefan Frittmann[1], Frank Endres[2], and Rolf Schuster[1] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Electrochemistry, TU Clausthal, Clausthal, Germany

The reversible molar heats, i.e., the Peltier heats of processes in the electrified double layer at an IL/Au(111) interface were measured via electrochemical microcalorimetry. The Peltier heat corresponds to the entropy change during electrochemical double layer charging. 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide was used as ionic liquid. We found a decrease of ΔRS by 143 J/(K*mol) between E vs. Pt = -0,9 V and +1,0 V and ΔRS = 0 for E vs. Pt = -0,25 V. ΔRS = 0 corresponds to the maximum of the double layer formation entropy SMax. We interpret SMax as the maximum of mixing entropy of cations and anions within a lattice gas model with negligible ionic interactions. As a consequence, SMax corresponds to the pzc (point of zero charge) of the system. In order to quantitatively explain the found magnitude of the S variations, one has to include entropy contributions from multiple layers.

O 21.5 Mon 17:45 MA 144

A thermodynamic approach on specific anion adsorption via electrochemical Microcalorimetry — •Marco Schönig and Rolf Schuster — Karlsruhe Institute of Technology, Karlsruhe, Germany

The understanding of specific adsorption is of fundamental importance for the description of the electrochemical double-layer. With electrochemical microcalorimetry we measured the reversibly exchanged heat during the anion adsorption/desorption process, which is directly correlated with the reaction entropy of the electrochemical process (1). Using this method we investigated the adsorption of halides (Cl-, Br-, I-) and oxoanions (SO42-/HSO4-, CLO4-) on Au(111) as a function of the surface polarization. For all systems the exchanged heat increased in the adsorption region of the respective anion. A possible explanation may be the configuration entropy of an anion lattice gas.

(1) J. M. Gottfried und R. Schuster. Surface Microcalorimetry. In: Surface and Interface Science. Weinheim, Germany: Wiley-VCH Verlag GmbH & Co. KGaA, 2016, S. 73-126

O 21.6 Mon 18:00 MA 144

Enhanced Photoanode Activity with Co-Fe Prussian blue as genuine Water Oxidation Catalyst — •Franziska Hegner[1], Núria López[1], José-Ramón Galán Mascarós[1], and Sixto Gimenez[2] — [1]ICIQ Tarragona — [2]INAM, Castellón

Catalysts based on Prussian blue analogues have shown high water-oxidation efficiencies with exceeding long-term stabilities. Moreover, their application as co-catalysts on well-known photoanode materials, such as α-Fe2O3 and BiVO4, has shown success. We studied the electrochemical behaviour, catalytic efficiency and impedance under light and electrical field conditions. Also transient absorption spectroscopy (TAS) is used to gain more information about the behaviour of the system. In addition, we employed various theoretical simulations based on hybrid Density Functional Theory, DFT, and evaluated their applicability. With a combination of theoretical, as well as experimental studies, the true catalytic function of cobalt-iron Prussian blue as a co-catalyst on light-absorbing semiconductors can be evaluated.

O 22: Overview Talk: Nian Lin

Time: Tuesday 9:30–10:15 Location: HE 101

Invited Talk O 22.1 Tue 9:30 HE 101

Metal-organic coordination on surfaces: towards complexity and functionality — •Nian Lin — Department of Physics, The Hong Kong University of Science and Technology

When multiple binding modes are present simultaneously in the metal-organic coordination self-assembly, the outcome becomes less predictable and novel phases may emerge. Here I discuss two examples. The first system is co-existing two-fold and three-fold modes of pyridyl-Cu coordination result in a demi-regular lattice which features local dodecagonal symmetry on a Cu(111) surface. This structure is thermodynamically robust and emerges solely when the molecular density is at a critical value. The second system involves Eu-carbonitrile coordination. Depending on ligand/metal stoichiometry, three-fold, four-fold, five-fold and six-fold coordination motifs can be formed on a Au(111) surface, resulting in various structures exhibiting irregular pores, square lattice, five-fold snub-square nodes structures, and hexagonal lattice. At a specific stoichiometry, the prevailing expression of five-fold and six-fold coordination nodes yields quasicrystalline tessellation. I will also discuss our recent efforts of synthesizing a pi-conjugated metal-organic system exhibiting a non-trivial topological band structure.

O 23: Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures II

Organizers: Sabine Maier, FAU Erlangen-Nürnberg; Meike Stöhr, University of Groningen
(Synopsis provided with part I of this session)

Time: Tuesday 10:30–13:00 Location: MA 004

Invited Talk O 23.1 Tue 10:30 MA 004
Electronic properties of functional organic compounds at surfaces: From zero- to two-dimensional — •Petra Tegeder — Ruprecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut

For improvement and optimization of the performance of organic molecule-based devices, comprehensive insight into the physical and chemical properties of the organic material at surfaces is necessary. I will present two case studies in which we investigated the electronic properties of organic/inorganic hybrid systems, namely graphene nanoribbons (GNRs) on gold surfaces and photochromic molecular switches on silicon. The GNRs are generated using a bottom-up approach based on a thermally activated and surface-assisted reaction of suitable precursor molecules. We studied the effect of N-doping on the energy level alignment. Additionally, we identified excitonic states in GNRs on gold surfaces. Incorporating photochromic molecules into organic/inorganic hybrid materials can lead to photoresponsive systems. In such systems, the second-order nonlinear optical properties can be controlled via external stimulation with light at an appropriate wavelength, which we could demonstrate.

O 23.2 Tue 11:00 MA 004
Identifying on-surface reaction products and orbital modifications with photoemission tomography — Xiaosheng Yang[1,2], Philipp Hurdax[3], Larissa Egger[3], Daniel Lüftner[3], Georg Koller[3], Petra Tegeder[4], F. Stefan Tautz[1,2], Michael G. Ramsey[3], •Peter Puschnig[3], and Serguei Soubatch[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, Germany — [3]Institut für Physik, Karl-Franzens-Universität Graz, NAWI Graz, Austria — [4]Ruprecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut, Germany

Dibromo-bianthracene (DBBA) has been shown to present an effective bottom-up strategy to fabricate atomically precise graphene nanoribbons on metal substrates. Here, we follow the thermally induced chemical reaction of DBBA deposited on Cu(110) to bisanthene ($C_{28}H_{14}$) by photoemission tomography. By comparison with density functional calculations, we can clearly identify a number of molecular orbitals associated with bisanthene including the filled LUMO. We unambiguously prove the chemical reaction taking place, clarify the molecular conformation and orientation before and after the reaction, and provide information on the charge state as well as on the electronic level alignment of the reaction product. Our work thus demonstrates the potential of photoemission tomography in monitoring complex reactions on surfaces.

O 23.3 Tue 11:15 MA 004
On-surface synthesis and characterization of atomic carbon wires — •Qiang Sun[1,2], Shiyong Wang[1], Wei Xu[2], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — [2]Interdisciplinary Materials Research Center, College of Materials Science and Engineering, Tongji University, Shanghai 201804, P. R. China

Carbon-based materials have received tremendous attention, fueled by successive discoveries of novel carbon allotropes such as fullerenes, carbon nanotubes, and graphene. Among others, linear chains of carbon atoms combine ultimately simple structures with intriguing properties. For instance, polyacetylene (PA) is the sp2 hybridized one-dimensional hydrocarbon chain. Owing to its simple chemical structure and exceptional electronic properties, PA is an ideal model system for understanding the nature of conducting polymers. Inspired by recent advances in the on-surface synthesis, we aim here at the synthesis of atomic carbon chains by the surface-assisted coupling of ethyne molecule (the simplest alkyne with two terminal alkynyl groups). Here, we report a successful on-surface synthesis of metalated carbyne chains by dehydrogenative coupling of ethyne molecules and copper atoms on a Cu(110) surface, which is characterized by high resolution STM, nc-AFM, and XPS combined with DFT calculations. Moreover, we have formed both cis and trans PA oligomers on the surface and investigated the electronic properties of trans PA chains through STS and ARPES measurements.

O 23.4 Tue 11:30 MA 004
Novel approach to grow 2D organic topological insulators by on-surface synthesis — •Fabian Schulz[1], Guoxian Zhang[2], Gerhard Meyer[1], Julian Chan[2], and Leo Gross[1] — [1]IBM Research - Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland — [2]University of Ottawa, 120 D'Iorio Hall, Ottawa ON, K1N 6N5, Canada

Honeycomb lattices comprising metal atoms with strong spin-orbit coupling connected by organic linker molecules are predicted to host topologically protected conducting edge states, thus giving rise to two-dimensional organic topological insulators (TIs) [1]. One possible route to create such structures experimentally are self-assembled metal-organic coordination networks grown on surfaces [2]. However, these networks are usually not fully covalently bonded, which would be desirable for realizing organic TIs. Even though there are several strategies to form covalent bonds by on-surface synthesis [3], those are rarely applied to grow metal-organic structures.

Here, the possibility to grow organic TIs by on-surface synthesis is explored. We use atomic force microscopy with CO-functionalized tips to study surface-assisted Ullmann coupling of tris(4-iodobenzene)bismuthine complexes on Ag(111). Our results reveal important challenges that need to be overcome in order for this novel approach to succeed.

[1] Z.F. Wang *et al.*, Nat. Commun. **4**, 1471 (2013).
[2] L. Dong *et al.*, Prog. Surf. Sci. **91**, 101 (2016).
[3] G. Franc *et al.*, Phys. Chem. Chem. Phys. **13**, 14283 (2011).

O 23.5 Tue 11:45 MA 004
Two-dimensional band structure in honeycomb metal-organic frameworks on epitaxial graphene — •Peter Liljeroth — Department of Applied Physics, Aalto University, Helsinki, Finland

Metal-organic frameworks (MOFs) are an important class of materials that present intriguing opportunities in, e.g., the fields of sensing, gas storage, catalysis, and optoelectronics. While there is a tremendous number of examples of three-dimensional, bulk, MOFs, synthesis strategies for two-dimensional (2D), monolayer thick MOFs are more limited. These systems are drawing growing interest as a promising platform for realizing designer materials with engineered electronic structures. The synthesis of 2D-MOFs is usually carried out on metal surfaces (e.g. Au, Ag, Cu), where it is difficult to access their intrinsic electronic properties.

We demonstrate synthesis of cobalt-dicyanobiphenyl and cobalt-dicyanoanthracene MOFs on epitaxial graphene and characterize their atomic geometry and electronic structure using atomic force microscopy (AFM), scanning tunneling microscopy and spectroscopy (STM and STS). We show the formation of a strongly coupled 2D electronic system in a MOF synthesized on a weakly interacting substrate. These results open the experimental path towards stand-alone MOF-based designer optoelectronic materials with complex, engineered electronic structures. The direct growth of 2D MOFs on graphene outlines possibilities of heterostructures with inorganic 2D materials with potential applications in sensors, catalysis and optoelectronics.

O 23.6 Tue 12:00 MA 004
Quantum dot coupling modification through barrier width in organo-halide arrays — •Jorge Lobo-Checa[1], Ignacio Piquero-Zulaica[2], Ali Sadeghi[3], Zakaria M. Abd El-Fattah[2], Toshihiro Okamoto[4], and Shigeki Kawai[5] — [1]Instituto de Ciencia de Materiales de Aragón (ICMA), CSIC-Univ. Zaragoza, Spain — [2]Centro de Física de Materiales, CSIC/UPV-EHU. San Sebastian, Spain — [3]Department of Physics, Shahid Beheshti Univ., Iran — [4]Department of Advanced Materials Science, Univ. Tokyo, Japan — [5]International Center for Materials Nanoarchitectonics, NIMS, Japan

Quantum dot (QD) arrays on surfaces, in the form of nanoporous networks, are candidates for studying fundamental physical phenomena such as 2DEG confinement. Tunability has been accomplished by varying the pore size, geometrical shape and molecule substrate interactions. Moreover, inter-dot coupling is validated by photoemission through the generation of new dispersive bands and modulated through thermodynamics and the condensation of guest elements.

Here, we validate the 2DEGs' modification through inter-dot barrier width by STM/STS/AFM, ARPES and extended model calculations. We engineer the inter-dot barrier width by substitution of a single atom in a haloaromatic compound and tune the confinement properties at each nanopore, affecting the degree of QD intercoupling both on bulk and thin Ag films alike [1].

[1] I. Piquero-Zulaica et al., Nat. Commun. 8, 787 (2017).

O 23.7 Tue 12:15 MA 004

Engineering the surface state of Au(111) by molecular patterning — Jun Li[1], •Nico Schmidt[1], Stefano Gottardi[1], Leonid Solianyk[1], Juan Carlos Moreno-Lopez[2], Zakaria M. Abd El-Fattah[3,4], Ignacio Piquero-Zulaica[5], Jorge Lobo-Checa[5], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Faculty of Physics, University of Vienna, Austria — [3]Faculty of Science, Al-Azhar University, Nasr City, Egypt — [4]ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, Spain — [5]Materials Physics Center, San Sebastian, Spain

The controlled tuning of material properties on the nanometer scale is a central goal in nanoscience. Artificial nanostructures can be built by STM in an atom-by-atom fashion. Corral structures built in this way were shown to confine the surface state electrons and locally modify the electronic surface properties. However, the manipulation process is impractical to change the properties of the entire surface. In contrast, molecular self-assembly offers the possibility to build well-ordered and defect-free nanostructures. By using different molecular building blocks, networks of different sizes and symmetries can be formed, which allows for tuning the electronic structure not only locally but also surface wide. Here, we report on tuning the electronic structure of Au(111) by adsorbing a porous molecular network made from 1,3,5-benzenetribenzoic acid molecules. With ARPES the formation of an artificial band structure based on surface state confinement was detected.

O 23.8 Tue 12:30 MA 004

The chemistry of artificial 2D atoms implemented at a metal-molecule interface — Aizhan Sabitova[1,2], Jeffrey Rawson[3,4,2], Ruslan Temirov[1,2], and •F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, Jülich, Germany — [3]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Germany — [4]Institute of Inorganic Chemistry, RWTH Aachen, Germany

Localising the hybrid metal-molecule interface state of PTCDA/Ag(111) at artificially patterned vacancies we form atom-like structures whose electronic states exhibit well-defined angular momenta, giving rise to direction-specific bonding interactions. These two-dimensional artificial atoms can be constructed into multinanometer-scale molecules whose wavefunctions exhibit features, such as sigma and π-bonding configurations, previously only attributed to natural molecular orbitals.

O 23.9 Tue 12:45 MA 004

Band structure of a metal-molecule interface state revealed by feature recognition scanning tunneling spectroscopy — •Aizhan Sabitova[1,2], Ruslan Temirov[1,2], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology

Adsorption of a monolayer of 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) on Ag(111) leads to emergence of an unoccupied free electron-like interface state [1]. Although the state is believed to be a hybrid of the Shockley surface state of Ag(111) and unoccupied molecular orbitals [1-4], the impact of the molecular overlayer has not been probed directly. Combining Fourier transform scanning tunneling spectroscopy with a new approach called feature recognition scanning tunneling spectroscopy (FR-STS) we map the dispersion of the PTCDA/Ag(111) interface state, resolve the gaps at the boundaries of its Brillouin zone, and image the corresponding standing wave band states. This information allows to reconstruct the scattering potential introduced by the molecular lattice.

[1] R. Temirov et al., *Nature* **444**, 350-353 (2006)
[2] C.H. Schwalb et al., *Phys. Rev. Lett.* **101**, 146801 (2008)
[3] M. Dyer and M. Persson, *New. J. Phys.* **12**, 063014 (2010)
[4] N.L. Zaitsev et al., *J. Exp. Theor. Phys.* **110**, 114-120 (2010)

O 24: Focus Session: Structure and Chemistry of Metal-Oxide Surfaces I

Time: Tuesday 10:30–13:15 Location: MA 005

Invited Talk O 24.1 Tue 10:30 MA 005

Modelling Photo-electrochemistry on Oxide Surfaces — •Harald Oberhofer — Technical University Munich, Garching, Germany

The role computer modelling plays today in understanding and optimising catalysts for photo-electrochemical reactions is undisputed. Yet, state of the art simulation approaches tend to rely on a number of assumptions and simplifications which—especially on oxide surfaces—may not be fully justified. For example, simulation of the all-important water oxidation reaction is mainly based on idealised surfaces and the computational hydrogen electrode (CHE) approach, which evaluates the thermodynamic feasibility of a catalyst looking at pathways where each hydrogen abstraction is coupled to the removal of one electron (PCET). The precise reactive site of the catalyst is thereby viewed as irrelevant, based on the premise of idealised surfaces. Yet, specifically on semi-conducting oxides both the assumption of PCET and of pristine, defect-free surfaces are not necessarily fulfilled.

In my presentation I will outline some of the steps necessary to augment theoretical approaches that so far have been geared towards the simulation of metal surfaces under ideal conditions to oxides under realistic conditions. There, the focus will lie on the nature of the reactive site—considering e.g. defects able to attract reaction-driving localised charge carriers—and the appearance of free energy barriers and their influence on reaction kinetics. Finally, for a realistic model of photo-electrochemical reactions occurring on the solid-liquid interface I will examine the role the solvent itself.

O 24.2 Tue 11:00 MA 005

Vanadium dioxide as high work function electrode — •Rongbin Wang[1,2], Keke Fu[1], Takayoshi Katase[3,4], Hiromichi Ohta[3], Steffen Duhm[1], and Norbert Koch[1,2] — [1]Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, China — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [3]Research Institute for Electronic Science, Hokkaido University, Japan — [4]Laboratory for Materials and Structures, Tokyo Institute of Technology, Japan

VO2 is a rather unique metal oxide as it exhibits a first-order metal-insulator (MI) transition from an insulating phase with monoclinic structure to a metallic phase with tetragonal rutile structure near 340K. The evolution of valence bands and core levels of VO2 thin films upon sputtering and annealing with or without residual O2 atmosphere was monitored by ultraviolet and X-ray photoemission spectroscopy. Sputtering and subsequent annealing in vacuum introduced lower oxidation state V species, leading to an increased density of V 3d derived bands close to the Fermi level. However, annealing under O2 results in stoichiometric VO2 with a high work function of up to 6.7 eV. In addition, the temperature dependent photoemission results illustrate the electronic structure evolution of VO2 during the metal-insulator transition.

O 24.3 Tue 11:15 MA 005

Atomic-scale structure of the Hematite α-Fe2O3(1-102) surface — •Florian Kraushofer, Zdenek Jakub, Magdalena Bichler, Jan Hulva, Martin Setvin, Michael Schmid, Ulrike Diebold, Peter Blaha, and Gareth S. Parkinson — Vienna University of Technology, Vienna, Austria

Hematite (α-Fe2O3) is a promising material for technological applications due to its abundance, low cost and chemical stability. Its 2.2 eV bandgap makes it potentially ideal as a photoanode for photoelectrochemical water splitting, but performance is hampered by slow reaction kinetics and the need for a significant overpotential.

To date, most surface science studies of α-Fe2O3 have focused on the (0001) facet, but preparing a stoichiometric surface under UHV conditions has proven problematic. Some authors have investigated the equally relevant (1-102) surface, and reported that a (1x1) and a reduced (2x1) termination can be reversibly prepared. Several models have been proposed for the (2x1) reconstruction, but as of now no scanning probe data exists to support or refute them.

Here we present an atomic-scale scanning tunnelling microscopy (STM) study of the (1x1) and (2x1) surfaces of α-Fe2O3 (1-102). The data acquired for the (1x1) termination support a bulk termination model, as predicted by previous publications, but STM and nc-AFM images of the (2x1) reconstruction are inconsistent with previously proposed models. We propose a new model based on ordered oxygen vacancies, the plausibility of which is confirmed by density functional theory (DFT) results.

O 24.4 Tue 11:30 MA 005

The (O12) surfaces of hematite and their interactions with water - a DFT study — •Magdalena Bichler[1], Florian Kraushofer[2], Zdenek Jakub[2], Gareth Parkinson[2], and Peter Blaha[1] — [1]Institute of Materials Chemistry, TU Wien — [2]Institute of Applied Physics, TU Wien

Hematite (α-Fe_2O_3) is abundant all over the world and might be used for several applications, including photo electrochemical water splitting.

We focus our study on the (1-102) surface of hematite (R-cut).For this surface two different terminations exist. On the one hand, there is a (1x1) bulk terminated stoichiometric surface, but at low O_2 pressure, a (2x1) reconstruction with missing oxygen atoms is formed.[1,2]

We carried out ab initio calculations by using the WIEN2k code[3]. Based on our DFT calculations, we present a new model of the (2x1) reconstruction, which is energetically more stable than the one that has been proposed so far[4] and agrees well with experiment (including STM simulations).

We also present our results of water adsorption on both surface terminations, including a (1x3) superstructure for water on the bulk terminated surface and discuss these data together with experimental findings.

[1] M. A. Henderson et al., Surf. Sci. 1998, 417, 66-81
[2] F. Kraushofer et al., JPCC, 2017, accepted
[3] http://www.wien2k.at
[4] M. A. Henderson, Surf. Sci. 2010, 604 1197-1201

Invited Talk O 24.5 Tue 11:45 MA 005

Potential-Specific Structure at the Hematite-Electrolyte Interface — Martin E. McBriarty[1], Joanne E. Stubbs[2], Peter J. Eng[2], Guido von Rudorff[3], Jochem Blumberger[3], and •Kevin M. Rosso[1] — [1]Pacific Northwest National Laboratory, Richland, WA, USA — [2]Argonne National Laboratory, Lemont, IL, USA — [3]University College London, Bloomsbury, London, England, UK

The structure of transition metal oxide interfaces with aqueous electrolyte regulates the reactions fundamental to (photo)electrochemical energy conversion and electrode degradation. Measurements that provide atomically precise structural models of ion and solvent arrangements are essential, but most rely on static conditions not operating conditions far from equilibrium. Using a novel cell, the structure of the hematite (α-Fe2O3) (1-102)-electrolyte interface was measured under controlled electrochemical bias using synchrotron crystal truncation rod X-ray scattering. At increasingly cathodic potentials, charge-compensating protonation of surface oxygen groups increases the coverage of bound water while adjacent water layers displace outwardly and became disordered. Returning to open circuit potential leaves the surface in a persistent metastable state. Thus, the flux of current and ions across the interface is regulated by multiple electrolyte layers whose structure changes in the applied potential. The study reveals the complex environment underlying the simplified electrical double layer models used to interpret electrochemical measurements and emphasizes the importance of condition specific structural characterization for properly understanding catalytic processes at these interfaces.

Invited Talk O 24.6 Tue 12:15 MA 005

Photoelectrochemistry on hematite: a first-principles view — •Anders Hellman — Department of Physics and the Competence Centre for Catalysis, Chalmers University of Technology, Sweden

Fe2O3 is an abundant n-type semiconductor that has excellent stability in neutral and alkaline electrolytes, but so far the reported solar-to-hydrogen conversion efficiency is far from the theoretical limit [1]. Major factors hampering the performance of Fe2O3 are high recombination rate and poor oxygen evolution kinetics.

In a recent publication, we showed that joining different oxides provide the possibility of control the recombination rate [2]. The mechanism relies on the formation of dipole-like electric fields at the interface which, depending on the field direction, attract or repel minority carriers from the interface. Here we investigate the built-in electric field generated at the interfaces of using first-principles methods. The results show how electronic band alignment and defects doping at the interface determine the direction and strength of the built-in field. We also comment how these can affect the oxygen evolution kinetics via the overpotential. Our understanding of the oxide nanostructures can be employed for designing and improving the performance of water-splitting photoelectrodes.

[1]: D. K. Bora, A. Braun, E. C. Constable, Energy Environ. Sci., 2013, 6, 407. [2]: B. Iandolo,B. Wickman, E. Svensson, D. Paulsson, and A. Hellman, Nano Lett., 2016, 16, 2381.

O 24.7 Tue 12:45 MA 005

Coverage-dependent Water Agglomerates on Fe_3O_4(001): Insights from Experiments — •Zdenek Jakub[1], Matthias Meier[1,2], Jan Hulva[1], Jiri Pavelec[1], Martin Setvin[1], Michael Schmid[1], Ulrike Diebold[1], Cesare Franchini[2], and Gareth S. Parkinson[1] — [1]Institute of Applied Physics, TU Vienna, Austria — [2]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Austria

The interaction between iron oxides and water plays a key role in many natural and technological processes. Recent water adsorption studies have found significant complexity on metal oxides, with reports of mixed-mode adsorption and hydrogen bonding. Here we present a multi-technique study of water adsorption on Fe_3O_4(001) surface. Quantitative temperature programed desorption (TPD) and X-ray Photoelectron Spectroscopy (XPS) experiments reveal four partially dissociated phases in the submonolayer regime, corresponding to coverages of 9, 8, 6 and 3 molecules per surface unit cell. These are investigated by non-contact atomic force microscopy (nc-AFM) with tip functionalized by CO molecule. This approach is highly convenient to study water agglomerates on metal oxide surfaces, and we can clearly demonstrate the existence of dimers and trimers, and a complex hydrogen-bonded network at lower coverage. These images can be further interpreted by DFT-based calculations, which will be presented in a separate talk.

O 24.8 Tue 13:00 MA 005

Transition metal clusters on tetragonal and monoclinic zirconia (ZrO_2) surfaces — •Zhiyu Zou, Peter Lackner, Sabrina Mayr, Ulrike Diebold, and Michael Schmid — Institute of Applied Physics, TU Wien, 1040, Vienna, Austria

Zriconia (ZrO_2) is widely used in heterogeneous catalysis, gas sensors and solid oxide fuel cells, where it is interfaced to transition metals. However, most investigations of ZrO_2/metal systems focus on powder samples, where surface-science techniques of high spatial (e.g. STM) or energetic (e.g. XPS) resolution are limited by the morphology and insulating nature of the samples.

We have developed a method to prepare clean, atomically flat ZrO_2 films (5-6 trilayers) with a precise control of phases (tetragonal or monoclinic) on Rh(111). The films are thin enough for STM and XPS measurements, yet show bulk-like crystallography. Transition metal (Rh, Fe, Au, Ag) clusters were deposited on both phases of ZrO_2. STM and XPS indicate Ag has the weakest interaction with the substrates, and Fe the strongest. In comparison with ultrathin (single-trilayer) ZrO_2 films on Pt_3Zr and Pd_3Zr[1], here Fe and Au are less affected by the underlying metallic substrate, resulting in higher density of Fe clusters and 3D cluster growth of Au. On tetragonal films, XPS shows small shifts of Zr3d and O1s core-level peaks; they shift much more on monoclinic films. Our work indicates the possibility of tailoring the electronic properties of transition metals by manipulating oxide support thickness and phases.

[1] J. J. Choi, et al. J. Phys. Chem. C 2016, 120, 9920

O 25: Plasmonics and nanooptics: Light-matter interaction, spectroscopy II

Time: Tuesday 10:30–13:00 Location: MA 041

O 25.1 Tue 10:30 MA 041

Influence of plasmon-induced hot-electrons on the lattice dynamics of graphene — •Marcel Weinhold, Sangam Chatterjee, and Peter J. Klar — Justus Liebig University Giessen, Institute of Experimental Physics I, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

The plasmon-induced excitation of hot-electrons holds an extraordinary potential for light harvesting up to the infrared region of the electromagnetic spectrum. Besides applications in photocatalysis, hot-carrier phenomena enable one to realize various semiconductor-based optoelectronic devices. Graphene is a promising material for utilizing plasmon-induced hot-electrons formed in gold nanoparticles. Since lattice dynamics have a major impact on the transport properties it is important to investigate the influence of gold nanostructures and the injected hot-carriers on graphene's vibrational modes.Therefore, we performed Raman-mappings across individual spherical gold nanoparticles deposited on graphene to both, generate hot-carriers in case of plasmon resonance and determine the corresponding Raman-spectra in order to obtain information on the change in lattice dynamics. We observe a systematic shift in the measured phonon-frequencies related to a coupling between the electronic and phononic system correlating with the applied laser power.

O 25.2 Tue 10:45 MA 041

Zooming in on the Surface: Numerics for Localization of Light on Coated Nanosponges — •Felix Schwarz and Erich Runge — TU Ilmenau, Institut für Physik und IMN MacroNano, 98693 Ilmenau

Nanoporous gold-nanoparticles (nanosponges) are an outstanding example for disorder-induced localization of light and huge field-enhancements, as shown by photoemission from long-lived, highly localized plasmons with unmatched excitation efficiencies [1]. Coated with nonlinear optical materials or quantum dots, these particles could serve as an easy-access tool for quantum optics and ultra-sensitive chemical sensors. However, as the nature of the localization and environment-induced changes remain poorly understood, the integration of these features proves difficult. Simulations are necessary to design structures with optimally tailored disorder properties for the given task. The challenge for these simulations is the required nanometer resolution to confidently resolve details of localized optical modes in thin coatings. We address this challenge by employing transformation optics to gain variable resolution in our simulation methods in addition to effective-medium approaches for domains where high resolution is not necessary. Results for various nanosponge geometries are presented and compared to recent experiments.

[1] G. Hergert et al., Light: Science & Applications (2017) 6, e17075 (2017)

O 25.3 Tue 11:00 MA 041

Vertically coupled complementary antennas as plasmonic nanosensors for the optical sensing of molecules in the mid infrared. — •Gökalp Engin Akinoglu and Michael Giersig — Freie Universität Berlin

Infrared plasmonic nanosensor (IR-PS) for surface enhanced infrared absorption spectroscopy are of great interest for the sensing of biological molecules. Here, we report on a novel design of a IR-PS based on vertically coupled complementary antennas (VCCAs). Fabrication of hexagonal ordered silicon Nanopillar arrays is realized by the combination of nanosphere lithography (NSL) and metal assisted chemical etching(MaCE). First, a hcp monolayer of polystyrene particles is plasma etched to form a non-close packed array which is used as a lithography template during metal deposition to obtain a metallic film with periodically ordered perforations. The latter undergoes MaCE to yield the hexagonaly ordered silicon Nanopillar arrays. Finally, the pillar array is coated with gold to produce a complementary plasmon active perforated film between the pillars and plasmon active disks on top of the pillars. We show that the optical response of the VCCAs is tunable through the geometric dimensions of the structure and we observe enhanced near field intensities from 10^2 up to 10^3.

O 25.4 Tue 11:15 MA 041

Dopant-Induced Plasmon Decay in Graphene — •Dino Novko — Freie Universität, Institut für Chemie und Biochemie, Berlin

Unique properties of graphene plasmons, such as their tunability and low decay rates, have opened up many new pathways to control the electromagnetic energy on the nanoscale. Thus far the experimental studies have reported on graphene plasmons with up to far- or mid-infrared energies, which is achievable with the standard field gating techniques. On the other hand, theory predicts that chemically doped graphene could support plasmon excitations up to telecommunication or even visible frequencies. Apart from that, the presence of dopant may influence electron scattering mechanisms in graphene and thus impact the plasmon decay rate. Here I show a first-principles study of these effects in single-layer and bilayer graphene doped with various alkali and alkaline earth metals [D. Novko, Nano Lett. (2017)]. I find new dopant-activated damping channels: loss due to out-of-plane graphene and in-plane dopant vibrations, and electron transitions between graphene and dopant states. The latter excitations interact with the graphene plasmon and together they form a new hybrid mode. The study points out a strong dependence of these features on the type of dopants and the number of layers, which could be used as a tuning mechanism in future graphene-based plasmonic devices.

O 25.5 Tue 11:30 MA 041

Electrodynamic simulations of 2D random spectrometer in the very near-infrared regime — •Paris Varytis[1,2], Dan-Nha Huynh[2], Wladislaw Hartmann[3,4], Wolfram Pernice[3,4], and Kurt Busch[1,2] — [1]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany — [2]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik & Photonik, Newtonstr 15, 12489 Berlin, Germany — [3]University of Münster, Institute of Physics, Wilhelm-Klemm-Str.10, 48149 Münster, Germany — [4]University of Münster, CeNTech - Center for Nanotechnology, Heisenbergstr. 11, 48149 Münster, Germany

Random spectrometers are suitable for portable sensing and efficient lab-on-a-chip functionality. Here, a comprehensive study of a random spectrometer based on 2D planar waveguiding structures in the very near-infrared and visible regime is presented. Our silicon-nitride-based integrated-optical layout is analyzed for both, TE and TM polarizations, by means of Mie theory and electromagnetic simulations using the Discontinuous Galerkin Time-Domain method. It is shown that in the diffusive regime the spectral resolution depends on single scattering properties such as the scattering efficiency and asymmetry parameter. Moreover, shifting from the near-infrared to the visible regime, the transport mean free path is reduced due to the stronger scattering and therefore enhanced effective optical path leads to higher spectral resolution.

O 25.6 Tue 11:45 MA 041

Modematching for helical plasmonic resonators — •Thorsten Feichtner[1], Katja Höflich[2], and Bert Hecht[1] — [1]Nano- Optics & Biophotonics Group, Department of Experimental Physics 5, Röntgen Research Center for Complex Material Research (RCCM), Physics Institute, University of Würzburg, Am Hubland, D-97074 2Würzburg, Germany — [2]Helmholtz Zentrum für Materialien und Energie Berlin, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany

Mode-matching is a novel theoretical approach for the description of optical coupling between a plasmonic device and multiple emitters or receivers [1]. Here we apply the method to describe the far-field coupling of nanometer-sized metal helices [2] to circular polarized light, proving the viability and flexibility of mode-matching. We also show that a 1D model is sufficient to describe qualitatively the complex scattering behavior of the helical plasmonic nano resonator.

[1] Feichtner, T., Christiansen, S., & Hecht, B. (2017). PRL, 119(21), 217401.

[2] Haverkamp, C., Höflich, K., Jäckle, S., Manzoni, A., & Christiansen, S. (2017). Nanotechnology, 28(5), 55303.

O 25.7 Tue 12:00 MA 041

Size dependence of coupling strength in hybrid plasmon-exciton nanoparticles — •Felix Stete[1,2], Phillip Schossau[1], Wouter Koopman[1], and Matias Bargheer[1,3] — [1]Institut für Physik & Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]Humboldt-Universität zu Berlin, School of Analytical Sciences Adlershof (SALSA), Unter den Linden 6, 10099 Berlin, Germany — [3]Helmholtz Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany

The coupling strength in plasmon-exciton core-shell nanoparticles is mostly measured by tuning the plasmon resonance and subsequently fitting the resulting anticrossing relation. However,the plasmon tuning is usually induced by changing the particle size or shape. In this case an investigation of the size dependence of the coupling strength is not possible.

We tune the plasmon resonance via layer-by-layer deposition of polyelectrolytes and thus without changing the size or shape of the particles [1]. With this technique we investigate plasmon-exciton nanorods of different sizes to reveal a strong dependence of the coupling strength on the particle size. For small nanoparticles the coupling becomes very strong and single emitter strong coupling is within reach.

[1] F. Stete et al., ACS Photonics, 4, 1669-1676, 2017

O 25.8 Tue 12:15 MA 041

Tunability of ferroelectric superlenses in the mid-infrared regime — •Lukas Wehmeier[1], Jonathan Döring[1], Stephan Winnerl[2], Susanne C. Kehr[1], and Lukas M. Eng[1] — [1]Technische Universität Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany

A superlens utilizes negative permittivity materials to create optical near-field images beyond the diffraction limit [1]. Ferroelectric perovskites are preferential candidates for designing superlenses at infrared (IR) wavelengths [2,3,4] since they intrinsically possess a negative permittivity close to a sample phonon resonance [5]. Nevertheless, superlensing is usually restricted to a narrow spectral range, only. This inherently screams for superlenses with optical tunability.

In this presentation, the evanescent image formed by bulk ferroelectrics and ferroelectric superlenses is inspected by applying scattering scanning near-field optical microscopy and spectroscopy. Particularly, we focus on the impact of the ferroelectric polarization; we will show, that polarization control via applying external electric fields provides a great potential for superlens tuning via local-scale optical anisotropies.

[1] J. B. Pendry, Phys. Rev. Lett. 85, 3966 (2000).
[2] T. Taubner et al., Science 313, 595 (2006).
[3] S. C. Kehr et al., Nat. Commun. 2, 249 (2011).
[4] S. C. Kehr et al., ACS Photonics 3, 20 (2016).
[5] S. C. Kehr et al., Phys. Rev. Lett. 100, 256403 (2008).

O 25.9 Tue 12:30 MA 041

Low-temperature scattering scanning near-field optical microscopy — •Tobias Nörenberg[1], Jonathan Döring[1], Denny Lang[1,2], Susanne C. Kehr[1], and Lukas M. Eng[1] — [1]Technische Universität Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany

Scattering scanning near-field optical microscopy (s-SNOM) is a powerful technique to probe the sample's local dielectric function far beyond the diffraction limit. Applications of s-SNOM include investigations of ferroelectric domains [1], plasmonic resonances [2], superlensing [3], just to name a few. Here, we present a s-SNOM LHe-cryostat setup that uniquely operates from 4 to 300 K [4]. Additionally, we combine this setup with a narrowband free-electron laser for mid-IR to THz sample excitation at $\lambda = 4 - 250\mu m$.

This presentation not only answers the technological challenges faced when implementing the low-temperature s-SNOM but, furthermore, also delineates the interesting scientific questions of in situ monitoring phase transitions in multiferroics, or differentiating microscopic phase coexistences and electronic excitations of prospective materials.

[1] J. Döring et al., Appl. Phys. Lett. **105**, 053109 (2014).
[2] P. Patoka et al., Opt. Express **24**, 1154-1164 (2016).
[3] S. C. Kehr et al., Nat. Comm. **2**, 249 (2011).
[4] D. Lang et al., Rev. Sci. Instrum., submitted (2017).

O 25.10 Tue 12:45 MA 041

Chemical enhancement contribution in surface enhanced Raman scattering — •Bo Liu[1], Peter Lemmens[1,2], Rainer Stosch[3], and Bernd Güttler[3] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]PTB, Braunschweig, Germany

In the fields of clinical chemistry, biotechnology, pharmacy, food industry and metrology, surface enhanced Raman scattering (SERS) is of enormous importance [1]. For a better insight into the complex light-matter interaction processes that lead to a signal enhancement, it is essential to experimentally distinguish and quantify the contributions from chemical (CMs) and electromagnetic mechanisms (EM) [2]. Here, we present an approach to estimate the relative CMs response of each Raman mode via analysing light induced degeneration of target molecules on designed metal/semiconductor SERS substrates [3]. Our work thereby provides a potential tool for understanding the CMs at the level of each mode. Work supported by DFG-RTG 1952/1 "NanoMet", Braunschweig-IGSM, and DFG-LE967/17-1. [1] Hampel, et al., Measurement Science and Technology (2017). [2] Kneipp, J. Phys. Chem. C 37, 21076 (2016). [3] Liu, et al., Nanotechnology 28, 195201 (2017).

O 26: Organic-inorganic hybrid systems and organic films III

Time: Tuesday 10:30–13:00 Location: MA 042

O 26.1 Tue 10:30 MA 042

Self-assembly and metal coordination of 1,4-bis(1h-tetrazol-5-yl)benzene on Ag(111) in vacuo — •Peter Knecht[1], Anthoula Papageorgiou[1], Bodong Zhang[1], Joachim Reichert[1], Nithin Suryadevara[2], Svetlana Klyatskaya[2], Mario Ruben[2], and Johannes Barth[1] — [1]Physics Department E20, Technical University of Munich, Garching D-85748, Germany — [2]Institute for Nanotechnology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen D-76344, Germany

A phenyl functionalized with two tetrazole moieties at para positions is promising for magnetically active metal-organic coordination networks [1]. This route can be potentially extended to polyphenyls, which would result in linear tuning of the separation of the magnetically active metal atoms in the network [2-3]. En route to prepare such surface supported networks, we investigated the self-assembly and metal coordination of 1,4-bis(1h-tetrazol-5-yl)benzene on the atomically smooth Ag(111) surface under UHV conditions. The molecular layers are prepared by organic molecular beam epitaxy. Scanning tunneling microscopy and X-ray photoelectron spectroscopy are used to investigate the assembly of the molecules and their chemical state. The coordination of the tetrazole moieties with the native Ag adatoms is observed after annealing to 160 °C, whereas coordination with magnetically active Fe3+ atoms is achieved upon codeposition and annealing to ~120 °C.

[1] Yan, Zheng et al. Chem. Commun. 48 (2012) 3960
[2] Schlickum, U. et al. Nano Lett. 7 (2007) 3813
[3] Kühne, Dirk et al. JACS 131 (2009) 3881

O 26.2 Tue 10:45 MA 042

Surface-activated spin-crossover of a low-spin Fe(II) complex probed by NEXAFS — •Sebastian Rohlf[1], Benedikt Flöser[2], Manuel Gruber[1], Matthias Kalläne[1], Simon Jarausch[1], Jan Grunwald[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

The controlled spin-state manipulation of Fe(II) coordination complexes by external stimuli is associated with pronounced changes in the electronic, magnetic, and structural properties and may be implemented in future spintronic devices. To preserve the functionality of spin-crossover (SCO) complexes in device-like environments, where the molecules are typically fragile, such as in direct contact to a metallic surface, their sterical stability needs to be enhanced. However, this generally leads to a decrease of the transition temperature below which bi-directional spin switching is possible. Here, we present a near edge X-ray absorption fine structure (NEXAFS) spectroscopy study of the stabilized SCO derivative $Fe(PyPyr(CF_3)_2)_2(phen)$ adsorbed on metallic surfaces. SQUID measurements showed that the high-spin state appears to be fully suppressed in the bulk complex. In contrast, our NEXAFS results indicate that in thin films the SCO functionality is activated in the vicinity of the surface. At low temperatures and during laser light irradiation, the studied complex exhibits an almost complete low-spin to high-spin state transition, which has not been observed for other bulk low-spin complexes so far.

O 26.3 Tue 11:00 MA 042

Mixed aliphatic self-assembled monolayers with embedded polar group — •Eric Sauter[1], Jean-Francois Morin[2], and Michael Zharnikov[1] — [1]Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [2]Departement de Chimie and Centre de Recherche sur les Materiaux Avancees (CERMA), Universite Laval, Quebec QC Canada G1 V 0A6

We studied structure, molecular orientation, morphology, and electrostatic properties of mixed self-assembled monolayers (SAMs) comprised of alkanethiolates with the dipolar ester group embedded into the alkyl backbone at two opposite orientations. The packing density and molecular orientation in these films were found to be similar to those of the "parent" single-component monolayers. Applying X-ray photoelectron spectroscopy (XPS) as a morphology tool, we could estimate that the mixed SAMs represent homogeneous intermolecular mixtures of both components, down to the molecular level, excluding existence of "hot spots" for charge injection. The analysis of the C 1s XPS spectra and the work function data suggests that the composition of the mixed SAMs fully mimicked the mixing ratio of both components in the solutions from which these SAMs were prepared, which suggests a minor role of the dipole-dipole interaction in the overall balance of the structure-building forces. Varying this composition, work function of the gold substrate could be tuned linearly, in controlled fashion within a 1.1 eV range, at the persistent chemical composition of the SAM-ambient interface.

O 26.4 Tue 11:15 MA 042

Adsorption energies of aromatic molecules from quantitative TPD — Stefan R. Kachel[1], Benedikt P. Klein[1], Janika Hochstrasser[1], Martin Schmid[1], Steffen Seiler[2], Bernd Meyer[2], and •J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Arguably the most important single parameter for the quantitative characterization of metal-organic interfaces is the adsorption energy, which can be determined by precision temperature-programmed desorption (TPD) experiments via the desorption activation energy. Such energies represent valuable benchmark data for comparison with computational studies and are important prerequisites for the further rational improvement of organic electronic devices, in which metal-organic interfaces occur at the contacts between electrode and semiconductor. Since many typical organic semiconductors are based on aromatic hydrocarbon backbones, we focus here on benzene and other aromatic model compounds and study their interactions with the (111) surfaces of Cu, Ag and Au. An advanced TPD setup with a cryoshroud housing around the mass spectrometer enables us to suppress desorbing molecules without a direct line-of-sight path between the surface and the ion source. The precise desorption energies obtained by detailed analysis will be compared with previous experimental and theoretical results.

O 26.5 Tue 11:30 MA 042

A simple modification of Grimme's D3 density functional dispersion correction scheme for more accurate adsorption energies of organic molecules on surfaces — •Steffen Seiler[1], Stefan Renato Kachel[2], Janika Hochstrasser[2], J. Michael Gottfried[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Fachbereich Chemie, Philipps-Universität Marburg, Germany

The semiempirical D3 dispersion corrections of Grimme [1] to density functional theory calculations are highly successful for predicting structural and energetical properties of molecular aggregates. However, when it comes to the adsorption of molecules on surfaces of solids, often a significant overbinding is observed. We will present a simple modification of the D3 scheme based on ideas of the older D2 version that significantly reduces the overbinding. The improvement will be demonstrated by comparing calculated binding energies of aromatic molecules and porphyrins on metal and oxide surfaces with recent data from state-of-the-art TPD experiments.

[1] S. Grimme, et al., J. Chem. Phys. **132** (2010) 154204.

O 26.6 Tue 11:45 MA 042

How Doping Influences the Nature of Charge Transfer at ZnO/F4TCNQ Interfaces — •Simon Erker and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

At inorganic/organic interfaces, charge transfer occurs in different forms depending on the nature of the substrate. On metals, where the adsorbate often hybridizes with the substrate, hybrid bands a formed. These lead to a uniform, fractional charging of the organic monolayer. In contrast, on insulating and inert substrates, charge is transferred as integer electrons, which leads to the coexistence of charged and neutral molecules on the surface. In this contribution, we study the charge distribution of F4TCNQ on ZnO using hybrid density functional theory. ZnO is particular interesting substrate, which allows to study the transition between these two mechanisms. Experimentally, it can be produced with high purity or doped until metallic conductance. Moreover, while the 000-1 surface is inert due to the presence of a hydrogen overlayer, the 10-10 surface exposes surface Zn atoms that can hybridize with organic adsorbates. Employing a recently developed approach to incorporate doping and the effect of long-ranged band bending into our calculations, we investigate the transition between fractional and integer charging as function of the doping concentration for the two different surfaces.

O 26.7 Tue 12:00 MA 042

F4-TCNQ and F6-TCNNQ Adsorbed on H-Si(111): Structure and Work-Function Changes. — •Haiyuan Wang, Svenja Janke, Sergey Levchenko, Mariana Rossi, and Matthias Scheffler — Fritz Haber Insitute of the Max Planck Society, Berlin, Germany

The tunability of hybrid inorganic/organic materials makes them promising candidates for more efficient photovoltaic and electronic devices. Even though the electronic properties of these materials critically depend on the structure of the interface, the latter is often poorly understood or characterized. Here we address model hybrid systems composed by the efficient electron acceptor molecules F4-TCNQ and F6-TCNNQ adsorbed on hydrogenated Si(111) surfaces [H-Si(111)]. We demonstrate how structural variations can lead to different electronic properties through a characterisation of these systems with density-functional theory, employing the HSE06 functional augmented with many-body van-der-Waals corrections [1]. We present exhaustive structure searches that show that F4-TCNQ and F6-TCNNQ lie flat on H-Si(111) at low coverages and become negatively charged. Interestingly, increasing the coverage to around 25% leads to a more stable structural motif with molecules standing at an angle to the surface. This motif is necessary to explain the work-function increase observed in experiment for the same system, which are performed in collaboration with T. Shultz and N. Koch (HU Berlin). This work is supported by SFB-951 project (HIOS).

[1] A. Ambrosetti et al., J. Chem. Phys. 140, 18 (2014).

O 26.8 Tue 12:15 MA 042

Structure and Property Prediction of Tetracene and Pentacene at H:Si(111): A Conceptual Picture for Hybrid Inorganic/Organic Systems — •Svenja Janke[1,2], Haiyuan Wang[1], Volker Blum[2], Sergey Levchenko[1], Mariana Rossi[1], and Matthias Scheffler[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Duke University, Durham, USA

Hybrid organic inorganic systems allow to combine the properties of organic and inorganic substances and hence open up a wide field for new materials with tunable properties. In particular, the organic compound offers a large range of functionalities and can be designed to be environmentally benign. As a key example of aromatic molecule-interface systems, we present a first-principles structure search and electronic-property investigation of pentacene (Pc) and tetracene (Tc) adsorbed at the hydrogenated Si(111) surface. The adsorption of single molecules is explored at different thin film coverage conditions with a structure search routine that includes grid- and random-structure search elements. This enables us to identify the most favorable orientation of the acene molecules and, using hybrid functionals, to investigate the level alignment between the organic and inorganic compounds with respect to the possibility of charge transfer: Single Tc and Pc molecules prefer to lie flat on the surface. For both organic molecules, the HOMO lies at the top of the valence band maximum allowing at best little charge transfer. For increasing coverage, we expect a transition to a dense geometry of standing molecules. This work is part of SFB-951 (HIOS).

O 26.9 Tue 12:30 MA 042

Optoelectronic Properties of Hybrid Systems of Inorganic Semiconductors and the Organic Semiconductor α-Hexathiophene — •Hannah Schamoni, Oliver Bienek, Felix Eckmann, and Martin Stutzmann — Walter Schottky Institut und Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Deutschland

The combination of organic and inorganic semiconductors is one promising approach towards new materials for applications like solar cells and light emitting devices, as they open up the possibility to benefit from the advantages of both material types. In order to identify the most promising hybrid systems, a detailed knowledge of the properties of the organic/inorganic interface is essential. In this work, thin films of the organic semiconductor α-hexathiophene are deposited on Si and SiC in an organic molecular beam deposition (OMBD) setup. The resulting hybrid systems are characterized amongst others by current-voltage and Kelvin Probe Force Microscopy measurements. On that basis, we discuss the influence of the choice of inorganic material on the optoelectronic properties of the hybrid systems. For example, the current-voltage output characteristics of the heterojunctions are found to depend on the doping type and strength of the inorganic substrate.

O 26.10 Tue 12:45 MA 042

Protoporphyrin IX functionalized GaN surfaces as a model system for photocatalytic hybrid devices — Felix Eckmann, •Jennifer Padberg, and Martin Stutzmann — Walter Schottky Institut und Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching

Efficient photocatalytic conversion of carbon dioxide into solar fuels constitutes an attractive option to reduce the problem of energy storage present in today's renewable energy technology. Although extensive research efforts have already been made, the conversion efficiencies and long-term stability of current devices are still far from feasible for large scale applications. In the current work, gallium nitride surfaces functionalized with protoporphyrin IX self-assembled monolayers are investigated as a model system to gain insights into future photocatalytic devices using similar functionalized surfaces. Sulfo-NHS activated protoporphyrin IX monolayers were created by adsorption from solution or by Langmuir-Blodgett deposition onto aminopropyltriethoxysilane-functionalized gallium nitride surfaces in order to create a chemisorbed monolayer. Thermally programmed desorption studies are carried out to gain information on the binding energy of the molecules on the surface. Polarized FTIR and AFM studies give indications on molecule orientation and layer morphology. Additionally, fluorescence spectroscopy and optical absorption spectroscopy highlight the changing optical properties accompanied by the transition from solved molecules to a chemisorbed solid monolayer.

O 27: Graphene: Electronic properties, structure and substrate interaction II (joint session O/TT)

Time: Tuesday 10:30–13:15 Location: MA 043

Invited Talk O 27.1 Tue 10:30 MA 043

Inside graphene devices — •Clemens Winkelmann[1], Sayanti Samaddar[1], Alessandro De Cecco[1], Hervé Courtois[1], Indra Yudhistira[2], Shaffique Adam[2], Vladimir Prudkovskiy[1,3], Claire Berger[1,3], and Walt de Heer[3] — [1]Univ. Grenoble Alpes / France — [2]NUS / Singapore — [3]Georgia Inst. of Technol. / USA

The electronic transport properties of devices are governed by microscopic physics which can often only be inferred indirectly from the former. By combining in situ transport and scanning probe experiments in graphene-based devices, we directly test the microscopic pictures used for predicting macroscopic transport properties.

The first part focusses on the charge puddles in diffusive graphene on a disordered dielectric substrate. Because of the linear dispersion relation in monolayer graphene, the puddles are predicted to grow near charge neutrality, a markedly distinct property from conventional two-dimensional electron gases. Using STM/STS on a gated single mesoscopic graphene device, we observe the puddles' growth as the Fermi level approaches the Dirac point. Self-consistent screening theory provides a unified description of both the macroscopic transport properties and the microscopically observed charge disorder.

The second part extends the above technique to a system with very little disorder, namely graphene nanoribbons grown on the sidewalls of steps of a SiC substrate. By performing STM (and the related scanning tunneling potentiometry technique) on such nanoribbons driven out of equilibrium, we gain novel insights into the extraordinary transport properties of graphene nanoribbons.

O 27.2 Tue 11:00 MA 043

Probing bulk and edge transport channels in sidewall graphene nanoribbons by dual-probe spectroscopy — •Johannes Aprojanz[1,2], Stephen Power[3,4], Anti-Pekka Jauho[4], Stephan Roche[3], and Christoph Tegenkamp[1,2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Institut für Physik, Technische Universität Chemnitz, Germany — [3]ICREA - Institucio Catalana de Recerca i Estudis Avancats, Barcelona, Spain — [4]Technical University of Denmark, DTU Nanotech, Center for Nanostructured Graphene (CNG), Lyngby, Denmark

The electronic confinement in graphene nanoribbons (GNR) leads to the formation of subbands as well as topologically protected edge states. GNR epitaxially grown on nanofacets of SiC mesa structures have shown fully spin-polarized ballistic transport signatures for probe spacings larger than 200 nm [1]. By means of a 4-tip STM/SEM contacts with even smaller probe spacings were realized. In this regime sudden jumps to plateaus of multiples of the conductance quantum e^2/h were observed using one blunt tip covering the entire GNR and one sharp tip gradually crossing the ribbon. We attribute these plateaus to edge and bulk transport channels, respectively. Based on tight-binding calculations these findings are explained by transversal electric fields which originate from distinct edge terminations on both sides of the GNR.

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

O 27.3 Tue 11:15 MA 043

Polycyclic molecules with geometrical frustration via pyrolysis on a metal — •Alexandre Artaud[1], Laurence Magaud[2], Kitti Ratter[3], Bruno Gilles[3], Valérie Guisset[2], Philippe David[2], Jose I. Martinez[4], Jose A. Martin-Gago[4], Claude Chapelier[5], and Johann Coraux[2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts Universität zu Kiel, Germany — [2]CNRS, Institut Néel, Grenoble, France — [3]Grenoble INP, SIMAP, Grenoble, France — [4]Materials Science Factory, Instituto de Ciencia de Materiales de Madrid-CSIC, Madrid, Spain — [5]CEA, INAC, PHELIQS, Grenoble, France

The geometry of molecules is a key to several of their properties. In graphene fragments, electron delocalization from one carbon sublattice to the other is frustrated for molecular shapes breaking the balance of sublattices. Optical, electronic, and magnetic properties emerge in this case, but the synthesis of such molecules remains challenging.

Here, a pyrolysis reaction catalysed by the surface of rhenium is investigated using scanning tunneling microscopy and density functional theory. This reaction known to form graphene is found to also yield graphene fragments consisting of well-defined, zigzag-edged polycyclic molecules, some of which have sublattice imbalance. However, they are found in metastable configurations, which is interpreted as a kinetic rather than thermodynamic control of their formation. Hence, metastable molecules are expectedly ubiquitous in graphene growth, and deleterious to achieve perfect graphene. Pyrolysis is conversely a promising route towards molecules with sought-after properties.

O 27.4 Tue 11:30 MA 043

Partial dislocations in bilayer graphene — •Reena Gupta[1], Heiko Weber[2], and Sam Shallcross[1] — [1]Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany — [2]Angewandte Physik, FAU Erlangen-Nürnberg, Staudtstrasse 7, 91058 Erlangen, Germany

We study the bernal stacked bilayer in the presence of symmetry lowering networks of partial dislocations. We find that the transport state of the bilayer is essentially determined by the structure of the partial dislocation network, which may result in both a minimal conductivity i.e., the appearance of a pristine bilayer, as well as an insulating phase [1]. We consider both an ideal model of straight partials, which reveals the essential physics, as well as more complex networks of wandering partials. Finally, we examine the topological edge states that exist at the partial dislocation edge, and examine their behaviour in the presence of an applied magnetic field.

[1] S. Shallcross et al., Nature Communications 8, 342 (2017).

O 27.5 Tue 11:45 MA 043

A topological edge state in the graphene twist bilayer — •Maximilian Fleischmann, Reena Gupta, Dominik Weckbecker, and Sam Shallcross — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany

The edge physics of graphene based systems is well known to be highly sensitive to the atomic structure at the boundary, with localized zero mode edge states found only on zigzag type terminations of the lattice. Here we demonstrate that the graphene twist bilayer supports an additional class of topological edge states, that (i) are found for all edge geometries (and thus are robust against edge roughness), (ii) occur at energies coinciding with twist-induced van Hove singularities in the bulk electronic spectrum and possess an electron density strongly modulated by the moiré lattice. Interestingly, these “moiré edge states” exist only for certain lattice commensurations and thus the edge physics of the twist bilayer is, in dramatic contrast to that of the bulk [1], not uniquely determined by the twist angle.

[1] S. Shallcross et al., Phys. Rev. B **87**, 245403, 2013.

O 27.6 Tue 12:00 MA 043

Structural study of the graphene/*n*-Ge(110) interface for nanoelectronic applications — •Julia Tesch[1], Fabian Paschke[1], Marko Wietstruk[2], Stefan Böttcher[2], Mikhail Fonin[1], Elena Voloshina[3], and Yuriy Dedkov[3,1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]SPECS Surface Nano Analysis GmbH, 13355 Berlin, Germany — [3]Department of Physics, Shanghai University, 200444 Shanghai, China

While graphene nanoelectronics show great promise to replace silicon-based technology in the future[1], the fabrication of graphene-based electronic units is accompanied by several drawbacks such as organic residue or metal contamination, defects and other transfer related issues. An alternative route to designing nanoscale device components is presented by epitaxial graphene growth directly on semiconducting substrates.

In order to shed light on the interactions at the graphene-semiconductor interface, we present local and macroscopic studies of graphene/Ge(110) regarding both structural and electronic properties investigated by means of low temperature STM/STS[2] as well as ARPES. The arrangement of dopants is discussed with respect to corrugation, Fermi velocity renormalization and doping level of graphene. Due to only a weak interaction between graphene and Ge(110) substrate, the characteristic linear dispersion of graphene is preserved, making it a viable candidate for device applications.

[1] Westervelt, Science 320, 324 (2008). [2] Tesch *et al.*, Carbon 122, 428 (2017).

O 27.7 Tue 12:15 MA 043

Landau-level spectroscopy of twisted epitaxial graphene multilayers on a metal substrate — •Sabina Simon[1], Elena Voloshina[2], Julia Tesch[1], Felix Förschner[1], Vivien Enenkel[1], Charlotte Herbig[3], Timo Knispel[3], Alexander Tries[4], Jörg Kröger[4], Yuriy Dedkov[1,2], and Mikhail Fonin[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Physics Department, Shanghai University, Shanghai 200444, China — [3]Institute of Physics II, University of Köln, 50937 Cologne, Germany — [4]Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Due to its potential in the development of new generation technologies, graphene remains the focus of many theoretical and experimental studies, principally when considering high-quality, large-scale epitaxial growth. In this work we investigate multilayered graphene systems epitaxially grown on Ir(111). Large patches of graphene twisted layers of high quality are fabricated upon atomic carbon intercalation underneath a continuous graphene sheet. By means of scanning tunneling spectroscopy in magnetic filed we study the evolution of the Landau-level spectra reflecting the variation of local electronic properties of the top graphene layer. We show that bilayers with large twist angles as well as twisted trilayers exhibit the electronic properties characteristic for a pristine graphene monolayer, pointing towards an effective decoupling of the top layer from the metal substrate. Complementary, we investigate changes in electronic properties of twisted graphene induced by subsequent alkali metal intercalation.

O 27.8 Tue 12:30 MA 043

Strong spin-orbit interaction in graphene/WSe$_2$ probed at local scale — •Mikhail Fonin[1], Felix Förschner[1], Fabian Paschke[1], Lena Stoppel[1], Julia Tesch[1], Yuriy Dedkov[2,1], and Andor Kormányos[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Department of Physics, Shanghai University, 200444 Shanghai, China

Deposition on transition metal dechalcogenide substrates allow to considerably modify the strength of spin-orbit interaction (SOI) in graphene, as shown in recent magnetotransport experiments [1,2]. Here we investigate structure and electronic properties of graphene on tungsten diselenide (WSe$_2$) by means of scanning tunneling microscopy and spectroscopy. In external magnetic field local spectroscopic measurements reveal pronounced Landau level sequences on graphene/WSe$_2$. Detailed analysis of the obtained tunneling spectra shows that each Landau level is split into subpeaks, where the splitting strength grows with increasing magnetic fields. We attribute the splittings to the manifestation of substrate induced SOI in graphene. A comparison of the experimental splitting strengths with the those yielded by a spin-dependent low-energy effective Hamiltonian allows the determination of the SOI coupling constants for the Rashba term and the so-called spin-valley coupling term. Furthermore, we map the real space fluctuations of the SOI coupling strength which correlate with the variations of local electronic potential.

[1] Z. Wang *et al.*, Nature Comm. **6**, 8339 (2015). [2] Z. Wang *et al.* Phys. Rev. X **6**, 041020 (2016).

O 27.9 Tue 12:45 MA 043

Origin of the band gap in Bi-intercalated graphene on Ir(111) — •Maxim Krivenkov[1,2], Dmitry Marchenko[1], Evangelos Golias[1], Jaime Sánchez-Barriga[1], Oliver Rader[1], and Andrei Varykhalov[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Str. 15, D-12489 Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Germany

We report a study of the structural and electronic properties of epitaxial graphene on Ir(111) intercalated with Bi. A novel structural phase of intercalated Bi was observed which is remarkably different from the phase reported earlier by Warmuth et al. [1]. This novel phase is more dense and, as seen by angle resolved photoemission spectroscopy, provides a quasifreestanding graphene with a very small band gap ($\sim$180 meV) and nearly ideal band structure without band replicas and electronic hybridization with the substrate. Furthermore, we demonstrate the possibility of fine tuning ($\pm$30 meV) of the band gap width in the Dirac cone by varying concentration of Bi.

To determine a possible origin of the observed band gap in Dirac point, we analyze the effect of structural corrugation on graphene band structure as well as interference effects in photoemission from graphene. The band gap was concluded to be of trivial nature and is ascribed to the breaking of sublattice symmetry of graphene.

[1] Warmuth et al. in Phys. Rev. B 93, 165437 (2016)

O 27.10 Tue 13:00 MA 043

Extremely flat band in bilayer graphene on silicon carbide — •Dmitry Marchenko[1], Daniil Evtushinsky[1], Vagelis Golias[1], Andrei Varykhalov[1], Thomas Seyller[2], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin fur Materialien und Energie GmbH — [2]Technische Universitat Chemnitz

In the present work we discover by angle-resolved photoemission an extremely flat band forming a strong 2D-extended van Hove singularity near the K point in bilayer graphene on SiC. We present a novel model for flat band formation in bilayer graphene and other bipartite lattices. Our finding implies that we can expect strong propensity towards a superconducting transition with high critical temperature.

O 28: Electronic Structure Theory: General I

Time: Tuesday 10:30–13:15 Location: MA 141

O 28.1 Tue 10:30 MA 141

ELPA-AEO: improvements to the eigensolver targetting electronic-structure theory — Andreas Marek[1], Hermann Lederer[1], Christian Carbogno[2], Matthias Scheffler[2], Lydia Nemec[3], •Christoph Scheurer[3], and Karsten Reuter[3] — [1]MPCDF, MPG, Garching — [2]Fritz-Haber Institut, MPG, Berlin — [3]Theoretical Chemistry, TUM, Garching

ELPA is a leading state-of-the-art library of massively parallel, highly scalable direct eigensolver routines.[1,2] It is heavily used by many application programs, e.g. from electronic-structure theory, such as FHI-aims, VASP, Quantum Espresso, or CP2K.

The ongoing ELPA-AEO project (BMBF 01IH15001) joins groups from numerical mathematics, computer science, high-performance computing, electronic structure theory, and theoretical chemistry and physics to develop algorithmic extensions and optimizations with an impact at the application level.[3] In this contribution we report on recent achievements and changes to the library. Application-level showcases with the electronic-structure code FHI-aims are presented and an outlook on new functionality is given.

[1] http://elpa.mpcdf.mpg.de
[2] A. Marek et al., J. Phys.: Condens. Matter 26 (2014), 213201
DOI: 10.1088/0953-8984/26/21/213201
[3] http://elpa-aeo.mpcdf.mpg.de

O 28.2 Tue 10:45 MA 141

An adaptive approach to solid-state QM/MM embedding — •Jakob Filser, Karsten Reuter, and Harald Oberhofer — Technische Universität München

QM/MM embedding in crystals [1,2] is a powerful approach to the simulation of non-periodic phenomena such as defects, as it eliminates issues like spurious self-interaction that are present in periodic boundary condition (PBC) supercell calculations. On the other hand, the performance of an embedding model depends crucially on the treatment of the QM/MM boundary and the long-range electrostatics in the MM region. Static setups that employ fixed effective core potentials (ECPs) to prevent charge leakage at the QM/MM boundary and fixed formal charges in the MM region are a common approach as both ECPs and formal charges are readily available [2]. However, such setups do not ensure correct reproduction of the electrostatic potential inside the QM region. We revisit this from an adaptive perspective, aiming to reproduce properties of reference density-functional theory PBC calculations in embedded defect-free supercells. Instead of fixed ECPs we optimize pseudo-potentials with an evolutionary algorithm to reproduce the charge distribution and energetics inside the QM region, providing a proof of concept that ECPs are indeed not the best choice for this purpose. For the MM region we propose a procedure to adapt the point charges to recover the long-range electrostatic potential.

[1] P. Sherwood *et al.*, J. Mol. Struct. - Theochem. 623, 1 (2003).
[2] D. Berger *et al.*, J. Chem. Phys. 141, 024105 (2014).

O 28.3 Tue 11:00 MA 141

A new design principle for embedded cluster models? Embedded-cluster calculations of surface oxygen vacancies at TiO_2. — •Matthias Kick, Karsten Reuter, and Harald Oberhofer — Technische Universität München

Surface oxygen vacancies, in particular their nature as charge trapping centers, play an important role for many oxide materials properties. However, addressing them with first-principles density-functional theory (DFT) computations remains a challenge. At least Hubbard corrected DFT+U is required to achieve an appropriate electron localization. At the same time, the large dielectric constant of polarizable oxides like TiO_2 leads to a strong polarization response. As a result supercells of increasing size are necessary in order to avoid spurious interactions between periodic images in case of charged defects, rendering the conventional periodic boundary condition supercell approach impractical. We combine the solid state (QM/MM) embedding functionality in FHI-aims with DFT+U, yielding a numerically most efficient approach to treat the aperiodic aspects at oxide surface. Systematic calculations of neutral and charged states of the surface oxygen vacancy at rutile TiO_2 (110) show that the shapes of the embedded cluster models are crucial for a proper description of surface phenomena. We assess this problem by proposing a new design principle for embedded clusters.

O 28.4 Tue 11:15 MA 141

On the Nature of Self-Consistency in Density Functional Theory — •Nick Woods[1], Mike Payne[1], and Phil Hasnip[2] — [1]Theory of Condensed Matter, University of Cambridge — [2]Condensed Matter Physics, University of York

Density functional theory (DFT) within the Kohn-Sham (KS) framework is a popular method for predicting the electronic structure of materials. The self-consistent field (SCF) method is an iterative procedure used to obtain a particle density that solves KS DFT (a 'self-consistent' particle density). Density mixing is a particular class of these methods which combines the particle densities of past iterations in such a way that drives each iterative density closer to solving KS DFT. We begin by discussing the various difficulties presented by solving KS DFT from the point of view of achieving self-consistency with density mixing. Then, we present a systematic study of various density mixing methods proposed in literature, which are examined by utilising a representative test suite of over twenty input systems. These example systems involve cases ranging from simple to nearly pathological. The purpose of this work is to highlight where and why certain schemes perform particularly well. Secondly, we discuss how model dielectrics can be used to accelerate and stabilise convergence of density mixing schemes, and propose a scheme whereby a density-dependent (inhomogeneous) model dielectric can be posited and used to assist convergence.

O 28.5 Tue 11:30 MA 141

The Kohn-Sham gap as example for an explicit density functional — •Martin Panholzer[1,3], Matteo Gatti[2,3], and Lucia Reining[2,3] — [1]Johannes Kepler University, Linz, Austria — [2]Laboratoire des Solides Irradies, Ecole Polytechnique, CNRS, CEA, Universite Paris-Saclay , F-91128 Palaiseau, France — [3]European Theoretical Spectroscopy Facility (ETSF)

It is well known that the density fully characterizes the ground state of a system. The use of the total energy as a functional of the density led to the usual implementation of Kohn-Sham(KS)-DFT. But other quantities, apart from the total energy, are rarely investigated. In this work we examine the KS-gap as a functional of the density. Numerically the inversion of the KS-equation is done iteratively. Different schemes are compared.

A purpose of the work is to investigate the sensitivity of a system to inaccuracies in the density, especially in view of a subsequent calculation of excited state properties. The KS-gap acts here as an easily accessible indicator.

We also use the density-functional formulation for the band gap to discuss the relation between the Kohn-Sham gap and the electron addition and removal gap.

O 28.6 Tue 11:45 MA 141

Calculation of molecular conductance "on the fly" for thousands of junction geometries — •Hector Vazquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

Single molecule circuits, where an electrical current is passed across a molecule placed between two electrodes, are ideal systems for studying a range of quantum phenomena[1]. Ab-initio transport calculations based on DFT-NEGF give a detailed description of transmission but their computational cost restricts this approach to a few structures.

In this talk I will describe an approximate method to calculate molecular conductance from a small cluster including the molecule. The reduced computational cost of this approximation enables the calculation of thousands of junction structures. When combined with Molecular Dynamics simulations, the evolution of junction structure and conductance can be simultaneously calculated. I will discuss this approximation to conductance and its implementation in the SIESTA code[2]. I will present results for several conjugated systems for tens of thousands of geometries[3] and analyze the relationship between molecular structure and conductance.

[1] T.A. Su, M. Neupane, M.L. Steigerwald, L. Venkataraman and C. Nuckolls, Nature Rev. Mater. 1 16002 (2016).

[2] J.M. Soler, E. Artacho, J.D. Gale, A. Garcia, J. Junquera, P. Ordejon, and D. Sanchez-Portal, J. Phys. Cond. Matt. 14, 2745

(2002).

[3] H. Vazquez, R. Skouta, S. Schneebeli, M. Kamenetska, R.Breslow, L. Venkataraman and M.S. Hybertsen, Nature Nanotechnol. 7 663 (2012).

O 28.7 Tue 12:00 MA 141

Band alignment at insulator/semiconductor interfaces through advanced electronic-structure calculations — •Thomas Bischoff, Igor Reshetnyak, and Alfredo Pasquarello — Chaire de Simulation a l'Echelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

Insulator/semiconductor interfaces are encountered in a broad variety of modern electronic devices. The precise understanding of their properties are of great fundamental and practical importance.

For an accurate description of such systems the band gaps of the consisting materials as well as their offsets must be predicted in an appropriate way. Unfortunately the calculation of these quantities in standard semi-local DFT suffer from the well-known self-interaction error. Advanced methods for electronic-structure calculation like the many-body perturbation theory and hybrid functionals can partially overcome this deficiency. However, these methods tend to position the band edges differently even when they give the same band gap [1]. This phenomenon which is not yet fully understood has direct implications on the band offsets in heterostructures [2].

In this work a representative set of insulator/semiconductor heterostructures is considered through various levels of theory. In particular, we focus on interfaces between materials with different bonding character.

[1] W. Chen et al., Phys. Rev. B 86, 035134 (2012)

[2] K. Steiner et al., Phys. Rev. B 89, 205309 (2014)

O 28.8 Tue 12:15 MA 141

Electronic and transport properties of the thermoelectric Mg_2X (X=Si,Ge,Sn) substitutional alloys — •Juan Guerra, Carsten Mahr, Marcel Giar, Michael Czerner, and Christian Heiliger — Justus Liebig University Giessen, Institut für Theoretische Physik, Giessen, Germany

Due to recent research interest in Mg_2X based binary substitutional alloy systems for thermoelectric applications, we present an ab initio description of electronic properties in the cases of X=Si, Ge, and Sn. We model these systems using the coherent potential approximation (CPA) implementation in the Korringa, Kohn and Rostoker Green's functions formalism in the full relativistic approach. Within this formalism, we use the Bloch spectral density function to obtain all physical observables. The change of structural parameters with composition deviates from Vegard's law and fits a cubic polynomial function. Relevant alloying effects on bands have been found thus affecting electronic states and effective masses. In the entire compositional range, we present a comprehensive analysis of some important physical quantities for transport, i.e., energy gaps (direct, indirect, and between the low-lying conduction bands), spin-orbit splitting energy, and parabolic band effective masses along different directions and at different symmetry points of the Brillouin zone.

O 28.9 Tue 12:30 MA 141

'Hartree-exchange' in ensemble density functional theory: guaranteed single-valued and maximally free from interactions — •Stefano Pittalis[1] and Tim Gould[2] — [1]CNR-Istituto di Nanoscienze, Via Campi 213A, I-41125 Modena, Italy — [2]Qld Micro- and Nanotechnology Centre, Griffith University, Nathan, Qld 4111, Australia

Ensemble density functional theory is, in principle, a promising framework to simplify the calculation of excitation energies of many-electron systems. But its application has been hampered by difficulties in calculating, and approximating, the exchange energy. We show that a better starting point is a *combined* 'Hartree-exchange' functional, $\mathcal{E}_{\rm Hx}[n]$, obtained as the right derivative of the universal ensemble density functional taken with respect to the coupling constant at vanishing interaction [Gould and Pittalis, *accepted* in Phys. Rev. Lett.]. This definition ensures that the resulting $\mathcal{E}_{\rm Hx}[n]$ is guaranteed single-valued – a basic prerequisite, which is at risk when dealing with densities from typical degenerate states – and is computable from a constrained minimization over valid non-interacting ensembles. Crucially, here the conventional restriction to single Slater determinants must be abandoned. The aforementioned definition can be finally restated – through use of the Schur-Horn theorem – into a practical expression which is also amenable to approximations. Specialized expressions from the literature can now be regarded as originating from the unifying approach presented here. Prototypical applications will be outlined, if time allows.

O 28.10 Tue 12:45 MA 141

Energy gaps of low-dimensional many-electron systems from Kohn-Sham quantities: Exchange-only approximations — •Alberto Guandalini[1], Carlo Andrea Rozzi[2], Esa Räsänen[3], and Stefano Pittalis[2] — [1]Dept. FIM, University of Modena and Reggio Emilia, Italy — [2]Center S3, CNR - Istituto Nanoscienze, Modena, Italy — [3]Dept. of Physics, Tampere University of Technology, Tampere, Finland

The electron addition energies of two-dimensional (2D) quantum dots are commonly obtained from the ground-state (gs) energies of systems with $N-1$, N, and $N+1$ electrons [1]. In this work we assess two alternative methods to calculate the addition energies. They resort to (a) the difference of the eigenvalues of the highest- ccupied Kohn-Sham (KS) orbitals for systems with N and $N+1$ electrons [2]; and (b) the KS gap plus the discontinuity of the exchange-correlation potential – through KS quantities for systems with N electrons [3]. While the original definition of the addition energy involves self-consistent gs calculations for three different systems, method (a) involves two of such calculations, and method (b) only one. At the exchange-only level, we analyze the performance of standard semi-local and (direct) potential approximations. We find that method (b) allows us to reduce the computational effort, yet maintaining the accuracy.

[1] Reimann and Manninen Rev. Mod. Phys. 74, 1283 (2002) [2] Capelle et al. Phys. Rev. Lett. 99, 010402 (2007) [3] Chai and Chen, Phys. Rev. Lett. 110, 033002 (2013)

O 28.11 Tue 13:00 MA 141

Importance of spin-orbit and on-site Coulomb interactions on the electronic structure and lattice dynamics of thorium and actinium — •Lukas Kyvala and Dominik Legut — VSB-Technical University of Ostrava, 17. listopadu 15/2172, 708 33 Ostrava, Czech Republic

We investigate electronic structure and lattice dynamics of thorium and actinium within density function theory. Recently, Actinium (Ac) shows excellent potential in radiotherapy and Thorium (Th) appears to be a suitable substitution for uranium in novel nuclear fuels. Therefore, we determined the effect of spin-orbit interaction (SOI) for the electronic, elastic, phonon and thermodynamic properties of number of Ac phases (*hcp*, *bcc*, *fcc*, and *sc*). Similarly, in the case of Th in addition to SOI we investigated also localized versus itinerant behavior of the f electrons. Therefore we applied so-called Hubbard parameter U in the range of 0.5-2 eV for the Th $5f$ electrons. Next, we calculated the elastic tensor by the linear-response method as implemented in VASP code to determine elastic constants (C_{ij}). Subsequently, the criteria of stability based on C_{ij} were evaluated. Subsequently, we calculated vibrational properties using the direct force-constant method as implemented in the PHONOPY code. Actinium phase transition is discussed within the quasi-harmonic approximation under temperature and pressure. Our calculated mechanical and thermodynamicl properties of Th are in good agreement with experimental data and for the Ac element serve as prediction. This work was supported by CSF grant No. 17-27790S and project No. CZ.02.1.01/0.0/0.0/16_013/0001791.

O 29: Metallic nanowires on semiconductor surfaces

Time: Tuesday 10:30–13:15 Location: MA 144

O 29.1 Tue 10:30 MA 144

Lattice dynamics of one-dimensional In chains on Si(111) upon ultrafast optical excitation — Tim Frigge, Bernd Hafke, Tobias Witte, Boris Krenzer, and •Michael Horn-von Hoegen — Fakultät für Physik und CENIDE, Universität Duisburg-Essen, 47057 Duisburg, Germany

The Indium induced (4x1) reconstruction on Si(111) is the prototype for 1D atomic wires at surfaces. At 130 K a metal-insulator transition to the (8x2) ground state takes place. A Peierls-like distortion causes periodicity doubling, opening of a band gap, and formation of a CDW. The non-equilibrium structural dynamics is studied by ultrafast RHEED with a fs-laser system in pump probe setup at temporal resolution better than 300 fs. Upon photo excitation the (8x2) ground state is driven in 350 fs to the (4x1) excited state as observed through the transient spot intensity changes. The transition is described in an accelerated displacive excitation scenario which relies on transient changes in the potential energy surface. The strong coupling between substrate and adsorbate is responsible for the sub-picosecond structural response by dephasing and damping the characteristic phonons in 1/4th of their oscillation period. Transient heating of the In atoms from 30 K to 80 K occurs delayed on a time scale of 2.2 ps. Thus the phase transition is driven by electronic entropy and not thermally.

O 29.2 Tue 10:45 MA 144

Infrared Spectroscopic Investigations of Charge Transfer in Quasi-1D Au-Induced Superstructures on Vicinal Silicon Surfaces — •Michael Tzschoppe, Christian Huck, Fabian Hötzel, and Annemarie Pucci — Kirchhoff Institute for Physics, Heidelberg University, Germany

Thermal evaporation of Au on vicinal silicon (*e.g.* Si(553)) under ultrahigh vacuum (UHV) conditions leads to atomic chain growth preferably along the step edges. During the experiments, the quality of the silicon surface, as well as the defined preparation of the atomic chains, are proven by reflective high energy electron diffraction (RHEED) measurements. We studied the plasmonic excitations of the metallic quasi-one-dimensional chains in the mid-infrared spectral region by Fourier transform infrared (FTIR) spectroscopy. By applying a model for excitations at low energies,[1] we are able to describe the spectrum and therefore to extract the one-dimensional free charge carrier concentration. In this talk, we will present how the free charge carrier concentration can be modified by doping the superstructures with organic molecules. For doping with C_{70}, the molecular adsorption leads to an increase of the plasmonic signal which can be attributed to an uptake of electrons by the C_{70} molecules adsorbed on the surface.

[1] Hötzel *et al.* Nano Lett. 15, 4155-4160 (2015)

O 29.3 Tue 11:00 MA 144

Light-induced phase transition in one-dimensional Indium wires — •Mariana Chavez-Cervantes, Razvan Krause, Sven Aeschlimann, and Isabella Gierz — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Strong Fermi surface nesting in one-dimensional wires drives Peierls transitions where a periodic lattice distortion opens up a band gap at the Fermi level. The In/Si(111)-(4x1) surface consists of quasi-one-dimensional indium wires which are metallic at high temperatures and become insulating below Tc~100K via a complex three-band Peierls transition assisted by interband charge transfer [1]. We study the light-induced insulator-to-metal phase transition using time- and angle-resolved photoemission spectroscopy (tr-ARPES), complementing recent investigations of the underlying lattice dynamics [2-3]. We observe closing of the band gap on a timescale (~500fs) that is a fraction of the amplitude mode period. The recovery time of the insulating state is found to be strongly fluence dependent with trapping in a metastable (4x1) phase at high fluences. We discuss the subtle role of the chemical potential [4] for both the temperature- and the light-induced phase transition.

[1]P. C. Snijders et al., Rev. Mod. Phys. 82, 307(2010)
[2]S. Wall et al., PRL 109,186101 (2012)
[3]T. Frigge et al., Nature 544, 207 (2017)
[4]E. Jeckelmann et al., Phys. Rev. B 93, 241407(R) (2016)

O 29.4 Tue 11:15 MA 144

Understanding solitonic excitations in the charge density wave ordered ground state of the In/Si(111) nanowire array from phonon theory — •Samad Razzaq[1], Stefan Wippermann[1], Tae-Hwan Kim[2], and Han-Woong Yeom[2] — [1]Max-Planck-Institut für Eisenforschung GmbH — [2]IBS Center for Artificial Low Dimensional Electronic Systems , University of Pohang

The Si(111)-(4x1)/(8x2)In atomic wire array is an extremely popular model system for one-dimensional electronic systems. It features a reversible temperature-induced metal-insulator transition into a charge density wave (CDW) ordered ground state. Solitonic excitations of the CDW and associated topological edge states are presently the focus of increasing attention. We carried out a combined *ab initio* and scanning tunneling microscopy (STM) study of solitonic phase defects in the In/Si(111) atomic wire array. We show how the solitonic CDW excitations can be modeled in terms of collective excitations of particular phonon modes. In conjunction with STM measurements, this phonon expansion approach allows us for the first time to determine the atomistic structure of the solitonic excitations. Due to the topological properties of the solitons and a strongly non-linear phonon-phonon coupling, these solitons interact in a deterministic way and are suitable for information processing. Financial support from the German Research Foundation (DFG), grant no. FOR1700 is gratefully acknowledged.

O 29.5 Tue 11:30 MA 144

Chiral topological solitons in the Si(111)-(8x2)In atomic wire array — Samad Razzaq[1], Tae-Hwan Kim[2], Han Woong Yeom[2], and •Stefan Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung — [2]Pohang University

The Si(111)-(8x2)In atomic wire array is a prototypical system featuring a one-dimensional charge density wave (CDW) formed at low temperature at the surface. As a consequence of CDW formation, the (8x2) phase exhibits a band inversion in the surface band structure. This system is therefore a candidate for a 1D topological insulator. Recent experimental findings indicate that the associated topological edge states take the form of chiral topological solitons. At present, these results, the associated concepts and their applicability with respect to atomic wires are intensely debated. In this talk we review the fundamental ideas behind the topological solitons in this system. We discuss how to understand the nature of the solitons and their interactions within phonon theory from first principles and provide some recent atomistic insights. Financial support from the German Research Foundation (DFG), grant no. FOR1700 is gratefully acknowledged.

O 29.6 Tue 11:45 MA 144

Quasi-ballistic transport through surface states of Ge(001)-c(4x2) demonstrated by two-probe STM measurements and multi-terminal fist-principles simulations — •Pedro Brandimarte[1], Marek Kolmer[2], Hiroyo Kawai[3], Thomas Frederiksen[1,4], Aran García-Lekue[1,4], Nicolas Lorente[5], Mads Engelund[5], Rafal Zuzak[2], Szymon Godlewski[2], Christian Joachim[6], Marek Szymonski[2], and Daniel Sánchez-Portal[1,5] — [1]DIPC, Spain — [2]NANOSAM-UNIWERSYTET JAGIELLO, Poland — [3]IMRE, Singapore — [4]IKERBASQUE, Spain — [5]CFM CSIC-UPV/EHU, Spain — [6]CNRS, France

Dangling-bond (DB) dimer wires on both Si and Ge(001):H substrates were predicted to be robust against electron doping and capable of sustaining ballistic transport [1]. The ability to fabricate high-quality DB-dimer wires on Ge(001):H was demonstrated and their transport properties were measured in atomic level using a two-probe scanning tunneling microscope (STM) setup [2].

We present a joint theoretical and experimental study of the electronic transport through DB-dimer wires on bare Ge(001) surfaces. First-principles calculations (DFT+NEGF [3]) of a four-terminal setup were carried out to simulate the two-tip experiment. Our results confirm the capability of the DB-dimer wires to sustain quasi-ballistic transport, and opens the possibility to their use as interconnects for atomic-scale devices fabricated on these surfaces.

[1] M.Engelund *et al.* JPCC **120**, 20303 (2016). [2] M.Kolmer *et al.* JPCM **29**, 444004 (2017). [3] N.Papior *et al.* CPC **212**, 8 (2017).

O 29.7 Tue 12:00 MA 144

Investigation of the phase transition in Si(553)-Au — •Frederik Edler[1,2], Ilio Miccoli[2], Herbert Pfnür[2], and Christoph Tegenkamp[1,2] — [1]Institut für Festkörperphysik, Technische Universität Hannover, 09126 Chemnitz — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover

Atomic wires are prototype 1D systems for studying fundamental aspects, e.g. charge density waves or dimensional crossover from a Fermi to a Luttinger liquid behavior. Recently, the Si(553)-Au system revealed a lot of attention because of their quasi-1D metallic structures with pronounced magnetic order, mimicking a quantum spin liquid [1]. However, up to now the phase transition of this system is not completely understood. By means of LEED and 4-tip STM, we investigated the surface structure and transport properties of Si(553)-Au as a function of temperature. LEED revealed an structural transition at T_C=100 K, i.e. the ×3 periodicity along the wires vanishes. In contrast, upon cooling the resistance increases at 120 K across the wires sharply by 2-3 and along the wires by one order of magnitude in transport experiments. By systematic variation of the intrinsic doping levels for the Si-substrates we were able to disentangle space-charge layer from surface state contributions. The latter transport channel indeed showed a metal insulator transition at 65 K. However, we clearly rule out a metal insulator transition which is associated to the phase transition of the ×3 reconstruction.

[1] B. Hafke et al., Phys. Rev. B. **94** (2016) p. 161403

O 29.8 Tue 12:15 MA 144

Control of plasmonic excitations in atomic arrays by adsorbates — •Zamin Mamiyev, Timo Lichtenstein, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany

Self-assembled atomic wires on vicinal Si surfaces serve the possibility to investigate fundamental properties of low-dimensional metallic systems. Electronic properties of such ultimate wires are strongly correlated with local structural motifs such as atomic arrangements, terrace width as well as inter- and intrawire distances. Therefore, the electronic correlation on such metallic wires is possible without direct contact with the atomic chains by the proximity effects. In this work modification of plasmonic excitations on Au-Si(hhk) surfaces by O_2 and H_2 adsorption has been studied via EELS-LEED with high resolution in energy and momentum. While the plasmon energy decreases by atomic hydrogen on Au-Si(553), gap opening is observed on Au-Si(557). Theoretical results show that hydrogen adsorption on Si step edges transfers charges to the metallic chains and increases band filling of Au-induced bands on Si(553), resulting in a metal-insulator transition. However, oxygen affects plasmon dispersion only on Au-Si(557), probably due to its higher chemical reactivity. Oxygen adsorption on Au-Si(557) is consistent with calculations that show that oxidation of adatom rows decreases the plasmon frequency. On the other hand, the excess amount of adsorbates induces disorder and finite propagation lengths.

O 29.9 Tue 12:30 MA 144

On the diffraction pattern analysis of bundled rare-earth silicide nanowires on Si(001) — Frederic Timmer, Jascha Bahlmann, and •Wollschläger Joachim — Fachbereich Physik, Universität Osnabrück, Osnabrück, Germany

Silicides of trivalent rare earth elemensts form nanowires (NW) on Si(001) surfaces caused by strain effects due to the different crystal structures of Si substrate and silide [1]. After intial growth of 2D wetting layers, single NWs are formed first while NW bundles appear during later stages. Since the structure of the NWs are not correlated, streaks emerge in diffraction pattern. The streaks, however, show some substructure after formation of NW bundles. Here, we report on the analysis of this structure based on the binary surface technique to obtain detailed information on the width distribution of single NWs and bundles of NWs as well as the distribution of bundle distances [2]. We apply our analysis on diffraction pattern from $DySi_2$ NWs recorded by SPA-LEED and compare the results with previous STM studies [3,4].

[1] M. Dähne, M. Wanka, J. Phys.: Condens. Matter 25 (2013) 014012.

[2] F. Timmer et al., J. Phys.: Condens. Matter 29 (2017) 435304.

[3] B.Z. Liu, J. Nogami, J. Appl. Phys. 93 (2003) 593.

[4] S. Appelfeller et al., Surf. Sci. 641 (2015) 180.

O 29.10 Tue 12:45 MA 144

A new atomic structure model for rare earth silicide nanowires on Si(001) — •Stephan Appelfeller[1], Jonas Heggemann[2,3], Tore Niermann[2], Michael Lehmann[2], and Mario Dähne[1] — [1]Institut für Festköperphysik, Technische Universität Berlin, Germany — [2]Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany — [3]Fachbereich Physik, Universität Osnabrück, Germany

Rare earth silicide nanowires on Si(001) are well known since 20 years. Soon after their discovery, their formation was explained by an atomic structure based on anisotropically strained hexagonal rare earth disilicide [1]. This univeral structure model was confirmed by scanning tunneling microscopy, with which only the surface of the nanowires is accessable.

Here, high-resolution transmission electron microscopy was utilized to analyze the cross-sections of Tb silicide nanowires with atomic resolution. For this purpose, the nanowires were passivated by an amorphous Si layer, which does not influence their inner structure [2]. As expected, hexagonal structural motives are found, but their orientation contradicts the accepted structure model of the nanowires. Thus, a new atomic structure model was developed based on these data as well as previous findings by scanning tunneling microscopy and low energy electron diffraction.

This work was supported by the DFG (FOR1700, E2).

[1] Y. Chen *et. al*, Appl. Phys. Lett. **76**, 4004 (2000).

[2] S. Appelfeller *et. al*, Appl. Phys. Lett. **108**, 013109 (2016).

O 29.11 Tue 13:00 MA 144

Optical characterization of rare-earth silicide nanostructures on vicinal Si(001) — •Sandhya Chandola[1], Eugen Speiser[1], Norbert Esser[1], Stephan Appelfeller[2], Martin Franz[2], and Mario Dähne[2] — [1]Leibniz-Institut für Analytische Wissenschaften ISAS e.V., Berlin, Germany — [2]Institut für Festkörperphysik, Technische Universität, Berlin, Germany

Rare-earth metals can interact strongly with Si(001) surfaces to form different types of silicide nanostructures such as wetting layers, nanowires as well as bundles of nanowires. Reflectance anisotropy spectroscopy (RAS) is used to monitor optically the growth evolution of Tb and Dy silicide nanostructures on vicinal Si(001) surfaces while STM is used to analyze their structural properties so as to directly relate the spectral signatures in RAS to the structural features. It is shown that the optical signatures of the different types of silicide nanostructures can be distinguished quite clearly with RAS due to their distinctive electronic properties associated with the structural units as observed with STM.

O 30: Focus Session: Phonon Polaritons: Opportunities for THz Nanooptics I

Time: Tuesday 10:30–13:00 Location: HE 101

Invited Talk O 30.1 Tue 10:30 HE 101
Recent Progress in Nonlinear Phononics and Josephson Plasmonics — •Andrea Cavalleri — Max Planck Institute for the Structure and Dynamics of Matter, Center for Free-Electron Laser Science (CFEL), Hamburg, Germany

In this talk I will discuss some recent applications of strong field THz and mid infrared pulses, which are used to control and to interrogate quantum materials. Especially, I will cover experiments in unconventionla superconductors and ferroelectrics.

Invited Talk O 30.2 Tue 11:00 HE 101
Femtosecond nanoscopy of collective excitations in semiconductors — •Markus A. Huber[1], Fabian Mooshammer[1], Markus Plankl[1], Leonardo Viti[2], Fabian Sandner[1], Miriam S. Vitiello[2], Tyler L. Cocker[1], and Rupert Huber[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]NEST CNR, 56127 Pisa, Italy

Far-field multi-THz studies are intrinsically limited in their spatial resolution to the scale of the probing wavelength by diffraction. Scattering-type scanning near-field optical microscopy (s-SNOM) overcomes this limitation by utilizing the electric near fields below the apex of a sharp metallic tip. Using ultrafast multi-THz s-SNOM we probe the transient, nanoscale dielectric functions of materials upon photoexcitation by femtosecond near-infrared pulses. We apply the system to investigate the plasmonic response in a single InAs nanowire, where ultrafast near-field tomography reveals the < 50 fs build-up of a surface depletion layer. Additionally, we resolve the oscillating electric near field on the wire surface directly in the time domain and demonstrate a spatial and temporal resolution of 10 nm and 10 fs, respectively. We also show that the insulator-to-metal phase-switching behavior in strained VO$_2$ nanobeams can be predicted via the local contrast of the pump-probe response at room temperature. Finally, we trace the evolution of photo-activated surface phonon-plasmon polaritons in custom-tailored black phosphorus/SiO$_2$ heterostructures on the nanoscale. These polaritons feature key elements for ultrafast control: ≈ 50 fs switch-on times and constant energy and momentum.

Invited Talk O 30.3 Tue 11:30 HE 101
Boron nitride nanoresonators for phonon-enhanced molecular vibrational spectroscopy at the strong coupling limit — •Marta Autore[1], Peining Li[1], Irene Dolado[1], Francisco J. Alfaro-Mozaz[1], Ruben Esteban[2,3], Ainhoa Atxabal[1], Fèlix Casanova[1,3], Luis E. Hueso[1,3], Pablo Alonso-González[4], Javier Aizpurua[2,5], Alexey Y. Nikitin[1,3], Saül Vélez[1,6], and Rainer Hillenbrand[1,3] — [1]CIC nanoGUNE, San Sebastián, Spain — [2]Donostia International Physics Center, San Sebastián, Spain — [3]IKERBASQUE, Basque Foundation fro Science, Bilbao, Spain — [4]Departamento de Física, Universidad de Oviedo, Spain — [5]Centro de Física de Materiales, San Sebastián, Spain — [6]Department of Materials, ETH Zürich, Switzerland

Surface enhanced infrared spectroscopy is a powerful strategy to increase the vibrational signature of molecules in FTIR spectroscopy, by means of the confined and enhanced field on the surface of plasmonic objects. Another option to enhance and confine IR light into subwavelength scale is to use phonon-polaritons (PhPs) in polar crystals or layered materials. In particular, the van der Waals material hexagonal boron nitride (hBN) hosts low-loss and high-momenta hyperbolic PhPs in the reststrahlen band (1360-1610 cm-1). We employ phononic antennas, hBN ribbons, to detect small amounts of organic molecules via IR transmission. The interaction between PhPs and molecular vibrations reaches the onset of the strong coupling regime. PhP nanoresonators thus could become a viable platform for sensing and active control of chemical reactivity and IR quantum cavity optics experiments.

Invited Talk O 30.4 Tue 12:00 HE 101
Ballistic surface plasmons in high mobility Dirac liquid of graphene — •Dmitri Basov — Columbia University, New York NY USA

Optical spectroscopies are an invaluable resource for exploring new physic of new quantum materials. Surface plasmon polaritons and other forms of hybrid light-matter polaritons provide new opportunities for advancing this line of inquiry. In particular, polaritonic images obtained with modern nano-infrared tools grant us access into regions of the dispersion relations of various excitations beyond what is attainable with conventional optics. I will discuss this emerging direction of research with two examples from graphene physics: i) ultrafast dynamics of hot photo-excited electrons [2]; and ii) ballistic electronic transport at low temperatures [3].

[1] D.N. Basov, M.M. Fogler and F. J. Garcia de Abajo *Polaritons in van der Waals materials*, Science 354, 195 (2016). [2] G. X. Ni, L. Wang, M. D. Goldflam, M. Wagner, Z. Fei, A. S. McLeod, M. K. Liu, F.Keilmann, B. Özyilmaz, A. H. Castro Neto, J. Hone, M. M. Fogler and D. N. Basov Nature Photonics 10, 244 (2016) [3] G. X. Ni, A. S. McLeod, L. Xiong et al. [submitted].

Invited Talk O 30.5 Tue 12:30 HE 101
Novel Materials and Approaches for Dynamic IR Nano-Optics — •Joshua Caldwell — Mechanical Engineering, Vanderbilt University, Nashville, TN USA

The field of nanophotonics is based on the ability to confine light to sub-diffractional dimensions. Up until recently, research in this field has been primarily focused on the use of plasmonic metals. However, the high optical losses inherent in such metal-based surface plasmon materials has led to an ever-expanding effort to identify, low-loss alternative materials capable of supporting sub-diffractional confinement. Beyond this, the limited availability of high efficiency optical sources, refractive and compact optics in the mid-infrared to THz spectral regions make nanophotonic advancements imperative. One highly promising alternative are polar dielectric crystals whereby subdiffraction confinement of light can be achieved through the stimulation of surface phonon polaritons within an all-dielectric, and thus low loss material system. Due to the wide array of high quality crystalline species and varied crystal structures, a wealth of unanticipated optical properties have recently been reported. This talk will discuss recent advancements from our group including the realization of localized phonon polariton modes, the observation and exploitation of the natural hyperbolic response of hexagonal boron nitride. Beyond this, methods to improve the material lifetime, realize active modulation and to induce additional functionality through isotopic enrichment and hybridization of optical modes will also be presented.

O 31: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Tuesday 10:30–13:00 Location: HL 001

O 31.1 Tue 10:30 HL 001

Control and prediction of molecular crystal properties by multilevel strategies — •Jan Gerit Brandenburg — London Centre for Nanotechnology, Department of Physics and Astronomy, University College London, 20 Gordon Street, London, U.K.

Computational material science is a dynamic and thriving area of modern scientific research. Approaches based on the fundamental laws of quantum mechanics are now integral to almost any materials design initiative in academia and industry, underpinning efforts such as the Materials Genome initiative or the computational crystal structure prediction [1]. I will present a hierarchy of quantum chemical methods designed for this purpose, in particular targeting molecular crystals and their property prediction. The methods range from high-level diffusion Monte-Carlo (DMC) to London dispersion inclusive DFT, and thus, cover many orders of magnitudes in computational efficiency [2,3]. I will demonstrate the application to the 6^{th} blind test for organic crystal structure prediction. Comparisons to other state-of-the-art methods indicate both success and remaining challenges in the recent method developments [4].

[1] S. L. Price and J. G. Brandenburg, *Molecular Crystal Structure Prediction*; Elsevier Australia, **2017**.

[2] A. Zen, J. G. Brandenburg, J. Klimeš, A. Tkatchenko, D. Alfè, A. Michaelides, **2017**, *submitted.*

[3] J. G. Brandenburg, E. Caldeweyher, S. Grimme, *Phys. Chem. Chem. Phys.* **2016**, *18*, 15519.

[4] A. M. Reilly, et al. *Acta. Cryst. B* **2016**, *72*, 439.

O 31.2 Tue 11:00 HL 001

Advances in first-principles and model spin Hamiltonian simulations of point defects in semiconductors for quantum sensors and computing — •Viktor Ivády — Department of Physics, Chemistry and Biology, Linköping University, 581 83 Linköping, Sweden — Wigner Research Center for Physics, Konkoly-Thege Miklós út 29-33, 1121 Budapest, Hungary

First principles simulations play a key role in understanding the physics of point defects in semiconductors, while model spin Hamiltonian approaches are traditionally used to interpret experimental spin dependent observations and describe the spin dynamics of point defects. The development of novel point defect applications, such as quantum bit (qubit) and single photon emitter applications for quantum information processing and quantum sensing, requires detailed understanding of spin-related couplings and addressability of localized defects states in the bath of delocalized electrons that calls for further development and implementation of theoretical tools. Here, I report on my contribution to this field that covers 1) first principles studies for identification of point defect based qubits and single photon emitters , 2) method development for the description of point defects with correlated electron states, 3) implementation of zero-field-splitting calculation for point defect based qubits, 4) development of model spin Hamiltonian approaches for the simulation of optical dynamic nuclear polarization process (ODNP) of point defects, and 5) spin dynamic simulation of existing point defect qubits. As an outlook, I discuss the requirements toward fully-ab initio point defect spin dynamic simulations.

O 31.3 Tue 11:30 HL 001

Recent advances in first-principles modelling of correlated magnetic materials — •Yaroslav Kvashnin — Department of physics and astronomy, Uppsala University, BOX 516, 75120 Uppsala

Most of modern first-principles electronic structure studies of correlated materials are based on a combination of density functional theory and dynamical mean field theory (DFT+DMFT).

Addressing magnetic materials within DFT+DMFT has certain peculiarities. There are two recipes one can follow: either to account for magnetism within the DFT functional or to introduce it entirely within the self-energy. Both approaches have their flaws and advantages, which are well-known for DFT+U, but are not often discussed for DFT+DMFT. In my talk I will present a systematic comparison of the two methods and demonstrate the evidences favouring the use of non-polarised functionals.

Next, I will demonstrate how the obtained electronic structure information can be used to simulate finite-temperature magnetic properties in real materials. I employ a so-called two-step approach. First, I map the system on a Heisenberg model and extract the effective exchange parameters Jij's from DFT+DMFT. Then the atomistic spin dynamics simulations are used to simulate magnon spectra and predict the magnetic ordering temperatures.

I will demonstrate the power of such an approach by showing a direct comparison with available experimental data for a wide range of different materials.

O 31.4 Tue 12:00 HL 001

A first-principles approach to hot-electron-induced ultrafast dynamics at metal surfaces — •Reinhard J. Maurer — Department of Chemistry, University of Warwick, Gibbet Hill Road, CV4 7AL Coventry, UK

Low-lying electronic excitations in metals, so-called hot electrons, couple efficiently to molecular adsorbate motion. In doing so, they give rise to a number of curious experimental observations. This includes picosecond-scale energy loss of molecular adsorbate vibration, highly inelastic atomic and molecular scattering from metal surfaces, and light-assisted molecular desorption and chemical transformations, recently coined "hot-electron chemistry". In this talk, I will present a first-principles treatment of hot-electron-induced molecular dynamics based on Density Functional Theory that correctly captures the magnitude and mode-specificity of hot-electron mediated adsorbate-substrate energy transfer [1]. Utilizing our efficient all-electron local-orbital implementation of hot-electron-induced frictional forces based on Time-Dependent Perturbation Theory, [2] I will show how we correctly capture vibrational relaxation in large-scale metal-mounted molecular catalysts as well as the energy loss and coupled electron-nuclear dynamics of small molecular adsorbates in both thermal and laser-heated conditions. [3] We scrutinize our approach in comparison to recent Sum-Frequency Generation (SFG) spectroscopy and molecular beam scattering experiments. [1] Phys. Rev. Lett. 116, 217601 (2016) ; [2] Phys. Rev. B 94, 115432 (2017); [3] Phys. Rev. Lett. 118, 256001 (2017);

O 31.5 Tue 12:30 HL 001

Temperature effects in spin-orbit physics from first principles — •Bartomeu Monserrat — University of Cambridge, UK — Rutgers University, USA

The spin-orbit interaction drives a number of physical phenomena, including the band inversion in topological insulators and the spin splitting of electronic bands in inversion asymmetric crystals. In this work, we study the effects of finite temperature on such spin-orbit physics, including both thermal expansion and electron-phonon coupling effects [PRB 92, 184301 (2015)].

First, we describe the temperature dependence of the inverted gap in topological insulators. We find that increasing temperature reduces the topological gap in the Bi2Se3 family of materials, and we predict a temperature-induced topological phase transition in Sb2Se3 [PRL 117, 226801 (2016)].

Second, we study the temperature dependence of the spin splitting of electronic bands in both inversion symmetric and asymmetric crystals. We predict a dynamical spin splitting in centrosymmetric crystals and characterise the associated phenomenology in the cubic perovskite CsPbCl3 [arXiv:1711.06274]. In inversion asymmetric crystals, exemplified by the bismuth tellurohalides, we find that increasing temperature suppresses the static spin splitting arising from the Rashba effect [PRM 1, 054201 (2017)].

O 32: Electronic structure of surfaces: Spectroscopy, surface states I

Time: Tuesday 14:00–15:30 Location: MA 004

O 32.1 Tue 14:00 MA 004

Soft x-ray spectroscopy of the plasma interface — •Florian Diekmann, Sebastian Rohlf, Felix Georg, Mathis Klette, Lisa Bauer, Matthias Kalläne, Thomas Trottenberg, and Kai Rossnagel — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel, 24098 Kiel, Germany

A better microscopic understanding of the fundamental electronic interactions between low-pressure plasmas and solid surfaces is presently hindered by the lack of experimental techniques that can probe both sides of the plasma interface on the relevant length and time scales: the electron- and ion-depleted space-charge region in front of the surface, i.e., the plasma sheath, as well as the electron accumulation layer in the surface region of the solid. Here, we show how to fill this void by combining synchrotron-based gas-phase and surface x-ray absorption spectroscopy into a novel experimental technique that provides direct spectroscopic information on the complete interface between low-pressure plasmas and solid surfaces. First *in situ* and *in operando* near edge x-ray absorption fine structure (NEXAFS) spectroscopy results on the plasma interface are presented for an Al_2O_3 substrate in contact with argon and neon plasmas.

O 32.2 Tue 14:15 MA 004

Photoelectron Momentum Microscopy with Large k-Field of View using Soft X-Rays — •Sergey Babenkov[1], Arndt Quer[2], Katerina Medjanik[1], Dmitry Vasilyev[1], Martin Ellguth[1], Florian Diekmann[2], Sebastian Rolf[2], Matthias Kalläne[2], Kai Rossnagel[2], Jens Viefhaus[3], Hans-Joachim Elmers[1], and Gerd Schönhense[1] — [1]JGU, Inst. für Physik, Mainz — [2]CAU, Inst. für Exp. und Angew. Physik, Kiel — [3]DESY, Hamburg, Germany

Time-of-flight k-microscopy at the high-brilliance soft X-ray beamline P04 (PETRA III) was employed for studying the electronic structure of several transition-metal dichalcogenides. Main emphasis was to maximize the field-of-view in k-space allowing to observe the k-patterns and circular dichroism (CDAD) texture in several repeated Brillouin zones (BZs) along $k_{x,y}$ (parallel) and k_z (perpendicular to the surface). CDAD patterns exhibit a rich texture, varying with k-vector in all directions and with photon energy. The dichalcogenides constitute an interesting intermediate case between true 2D systems as discussed in early CDAD work [1] and bulk systems as studied recently [2]. Varying k_z in small steps via the photon energy (from 290 to 370 eV, with ca. 5 eV increment) reveals strong redistributions of spectral weight of the Fermi-surface pockets at Γ, *M*, *M'* between the first and the repeated BZs along $k_{x,y}$. This is accompanied by pronounced changes in the CDAD texture. The variation with k_z allows to quantify the size of the quasi-3D Fermi surface via tomographic k-space mapping.

[1] G. Schönhense, Phys. Scripta **T31**, 255 (1990); [2] O. Fedchenko et al., submitted (2017)

O 32.3 Tue 14:30 MA 004

Probing the electronic structure of atomically-thin carbon nitride nanosheets photocatalytsts by soft X-ray spectroscopies — •Jian Ren[1,2], Nannan Meng[3], Iver Lauermann[4], Bin Zhang[3], and Tristan Petit[1] — [1]Institute of Methods for Material Development, Helmholtz-Zentrum Berlin für Materialen und Energie GmbH, Germany — [2]Department of Physics, Freie Universität Berlin, Germany — [3]Department of Chemistry, Tianjin University, China — [4]PVcomB, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Polymeric carbon nitride (PCN) is a promising earth-abundant 2D material for solar energy conversion. Optical, electronic, and chemical properties of PCN materials can be manipulated by changing the size, composition, dimension and shape of their reactive (nano)domains. Exfoliation is a promising strategy to enhance PCN photocatalytic performance via preparation of ultrathin nanosheets. In this work, the electronic structures and surface chemistry of the oxygen- and amino group decorated atomically-thin PCN nanosheets, as determined from infrared, soft X-ray absorption and ultraviolet photoemission spectroscopies, will be detailed. A special attention will be given to determine the structure-performance relationship of PCN photocatalysts by comparing the photocatalytic activity of these different materials with their electronic and surface chemical properties. These measurements were performed at the BESSY II synchrotron in Berlin. Synchrotron radiation-based soft X-ray spectroscopies have become powerful techniques to investigate the electronic structure of 2D materials.

O 32.4 Tue 14:45 MA 004

Layer thickness dependence of the Kondo temperature in the surface alloy $CePt_5$ on Pt(111) — •Katharina Treiber, Philipp Eirich, Chul Hee Min, and Friedrich Reinert — Experimentelle Physik VII, Universität 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]. This inelastic scattering process leads to a reduction of the f-level occupancy to $n_f < 1$. This is reflected in the Ce *3d* core levels. The spectral weight of their spin orbit split *3d 3/2*- and *5/2* peaks is redistributed on six peaks mirroring the f-level occupation [2]. Previous studies have shown that the $CePt_5$ surface alloy appears in a variety of different phases depending on Ce coverage and post annealing procedure [3]. XAS and XMCD studies recently suggested a change of the correlation strength throughout those different phases [4].

In this contribution we examine the electronic structure of the different phases regarding their various structural changes, by XPS and ARPES. We explore the hybridization strength and effective occupancy of the *4f*-electrons as a function of temperature, probing depth and $CePt_5$ layer thickness. This provides us with an opportunity to tune the strength of the electronic correlation in $CePt_5$ on Pt(111). [1] M. Garnier *et al.*, Phys. Rev. B **56**, R11399(R), (1997) [2] O.Gunnarsson, K. Schönhammer, Phys. Rev. B **28**, 8, (1983) [3] J. Kemmer *et al.*, Phys. Rev. B **90**, 195401 (2014) [4] C. Praetorius *et al.*, Phys. Rev. B **92**, 045116, (2015)

O 32.5 Tue 15:00 MA 004

Electronic structure of V- and Cr-doped $(BiSb)_2Te_3$ thin films. — •Sonja Schatz[1], Can Raphael Crespo Vidal[1], Thiago R. F. Peixoto[1], Hendrik Bentmann[1], Martin Winnerlein[2], Steffen Schreyeck[2], Charles Gould[2], Karl Brunner[2], Laurens W. Molenkamp[2], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Experimentelle Physik III, Universität Würzburg, D-97074 Würzburg

Magnetic topological insulators have received large interest in recent years, as they realize the long-sought-after quantum anomalous Hall effect. In particular, V- anc Cr-doped $(Bi_xSb_{1-x})_2Te_3$ thin films have been reported to exhibit an insulating ferromagnetic ground state and a quantum anomalous Hall phase at low temperatures. The macroscopic magnetic properties of these films vary depending on dopingtype (V vs. Cr) [1] and on the host stoichiometry parameter x. Here, we present our investigations on the electronic structure in dependence of these parameters by resonant photoelectron spectroscopy at the $2p$ absorption edges. We find that V $3d$ states are located at the Fermi level E_F, while for Cr the $3d$ states shift towards higher binding energies and show a vanishing density of states at E_F. We discuss possible implications on the nature of the ferromagnetic interactions in this material class.

[1] C. Z. Chang *et al., Nature Materials* **14**, 473 (2015).

[2] T. Peixoto *et al., Physical Review B* **94**, 195140 (2016).

O 32.6 Tue 15:15 MA 004

Systematics of electronic and magnetic properties in the transition metal-doped quantum anomalous Hall platform Sb_2Te_3 — •Johannes Jung[1], M. Bode[1], P. Sessi[1], S. Schatz[1], T.R.F. Peixoto[1], H. Bentmann[1], F. Reinert[1], A. Barla[2], M.F. Islam[3], A. Pertsova[4], A. Balastky[4], and C. M. Canali[3] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, Würzburg, Germany — [2]Istituto di Struttura della Materia, Trieste, Italy — [3]Department of Physics,Linnaeus University, Kalmar, Sweden — [4]Nordita, Stockholm University, Sweden

The quantum anomalous Hall effect has been reported to emerge in magnetically doped topological insulators. While its phenomenological description is quite clear, its microscopic origins are far from being completely understood and controlled. Here, we provide a systematic characterization of the most prominent QAHE platform: transition metal-doped Sb_2Te_3. By combing complementary experimental techniques (STM/STS/resPES/XMCD) with ab-initio theory, we analyze how $3d$ dopants (V, Cr, Mn, Fe) impact the electronic and magnetic properties. Our results reveal that the fate of the topological surface state strongly depends on the specific character of the $3d$ impurity. In particular, (i) the single-ion magnetic anisotropy, which controls the magnetic gap opening and its stability, can vary from in-plane to out-of-plane depending on the dopant; (ii) the emergence of impurity resonances close to the Dirac point can give rise to new bands, significantly altering the Sb_2Te_3 electronic structure. Overall, our results provide general guidelines for the realization of a robust QAHE.

O 33: Semiconductor substrates: Structure, epitaxy and growth

Time: Tuesday 14:00–15:15 Location: MA 005

O 33.1 Tue 14:00 MA 005

Growth, structure and morphology of tin deposited on Silicon and germanium surfaces — •Nicolas Braud, Thomas Schmidt, and Jens Falta — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

SnGe is expected to play an important role in optoelectronic and in future Ge device modules integrated into CMOS technologies due to its potentially indirect to direct band gap transition and its higher carrier mobility compared to Ge.
Here we present the investigation of the initial growth and adsorption of Sn on Si(001), Ge(001) and on a compressivly strained Ge wetting layer grown on Si(001) by means of low energy electron diffraction and microscopy.
After the deposition of Sn on Si(001) at elevated temperature, a (2×N)-reconstruction was observed. The N-fold periodicity evolved immediatliy after the beginning of the deposition and decreased from $N\approx50$ to N=4.6 with increasing Sn coverage. For Sn on a strained Ge wetting layer a similar behavior was observed. Also for growth of Sn on bulk Ge(001), an N-fold superstructure was observed. However, the minimum value of N=6.4 was higher than on bulk Si and than on strained Ge/Si.
This leads to the conclusion that strain ist the driving force for these reconstructions.

O 33.2 Tue 14:15 MA 005

Study of As-modified Si(100) surfaces for III-V-on-Si heteroepitaxy in CVD ambient — •Agnieszka Paszuk, Oliver Supplie, Manali Nandy, Anja Dobrich, Peter Kleinschmidt, and Thomas Hannappel — Institute of Physics, Technische Universität Ilmenau, Germany

III-V heteroepitaxy on Si(100) holds promise for low cost, high-efficiency optoelectronic devices. In polar-on-nonpolar epitaxy, it is crucial to prepare Si(100) surfaces with double-layer (DL) steps in order to avoid antiphase domains, which can significantly reduce the efficiency of the device. Here, we employ vicinal and almost exactly oriented Si(100) substrates relevant for photovoltaic and CMOS applications, respectively. We study the interaction of Si(100) surfaces with Arsenic, which is present in most application-relevant III-V MOCVD reactors, supplied either directly via the TBAs precursor or indirectly as background As_x. The entire process is controlled *in situ* by reflectance anisotropy spectroscopy (RAS) and the obtained spectra are benchmarked by UHV surface analytic techniques. We show that specific processing routes enable control of the dimer orientation on Si(100):As surfaces and we demonstrate low-offcut *single-domain* Si(100):As surfaces with regular, true DL steps. The process conditions to obtain a DL stepped surface depend on the offcut magnitude. We found that both As coverage and dimer orientation on the Si surface contribute to the RA spectral line-shape, which opens perspectives to fine-tune the surface structure as desired for further III-V growth.

O 33.3 Tue 14:30 MA 005

Molecular dynamics simulations of vapor-deposited amorphous selenium — •Julian Schneider[1], Amirhossein Goldan[2], and Anders Blom[1] — [1]Synopsys QuantumWise , Copenhagen, Denmark — [2]Department of Radiology, Stony Brook University, Stony Brook, USA

The structure of amorphous selenium is clouded with much uncertainty and contradictory results regarding the dominance of polymeric chains versus monomer rings. Here, we present Molecular Dynamics simulations using the VirtualNanoLab (VNL) and Atomistix ToolKit (ATK) with the ATK-ForceField module [1] to elucidate atomistic details of the structure of vapor-deposited amorphous selenium and compare these to melt-quenched amorphous selenium. We find pronounced differences depending on the preparation procedure, suggesting that the as-deposited structures predominantly consist of a ring-like topology, whereas melt-quenched samples reveal a more chain-like structure [2]. Although the exact topological details of the atomic structure of amorphous selenium is difficult to access via experimental techniques, these findings are indirectly corroborated by analyzing the conversion of vapor-deposited samples between various metastable structures.

[1] J. Schneider et al. "ATK-ForceField: A new generation molecular dynamics software package" Modelling Simul. Mater. Sci. Eng. 25, 085007 (2017)

[2] A.H. Goldan, C. Li, S.J. Pennycook, J. Schneider, A. Blom, and W. Zhao, "Molecular structure of vapor-deposited amorphous selenium" J. Appl. Phys. 120, 135101 (2016)

O 33.4 Tue 14:45 MA 005

Delta-doped phosphorus layers in silicon — •Ann-Julie Utne Holt[1], Sanjoy Mahatha[1], Raluca-Maria Stan[1], Frode Sneve Strand[2], Thomas Nyborg[2], Alex Schenk[2], Simon Phillip Cooil[3], Marco Bianchi[1], Philip Hofmann[1], Justin Wells[2], and Jill Miwa[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), University of Aarhus, 8000 Aarhus C, Denmark — [2]Department of Physics, Norwegian University of Science and Technology (NTNU), N-7491 Trondheim, Norway — [3]Institute of Mathematics and Physics, Aberystwyth University, Aberystwyth SY23 3BZ, UK

A δ-layer is a buried, high-density, doping profile in a semiconductor host. Such a doping profile may give rise to the formation of a two-dimensional electron gas (2DEG) in the dopant layer [1]. Phosphorus δ-layers in silicon combined with scanning tunneling microscope lithography have led to the fabrication of functional atomic scale devices [2]. By creating such δ-layers, varying in thickness from an atomically sharp doping profile to a 4.0 nm thick dopant layer, the effect of quantum confinement on the electronic structure of a induced 2DEG was studied using angle-resolved photoemission spectroscopy. The location of theoretically predicted, but experimentally undiscovered, quantum well states known as the Δ -manifold was revealed, validating density functional theory calculations developed for describing these δ-layer systems. Verification of these states contributes to the development of accurate models describing the electronic behavior of δ-layer derived devices.

O 33.5 Tue 15:00 MA 005

In situ study of AlxGa1-xP nucleation on As-modified Si(100) 2° surfaces — •Manali Nandy, Agnieszka Paszuk, Anja Dobrich, Oliver Supplie, Peter Kleinschmidt, and Thomas Hannappel — TU Ilmenau, Gustav-Kirchhoff-Straße 5, 98693 Ilmenau

Epitaxial growth of III-V materials on Si substrates is promising for cost-effective, tandem solar cells with high photovoltaic conversion efficiency. In order to avoid antiphase domains during polar-on-non polar heteroepitaxy, an atomically ordered, As-modified double layer (DL) stepped Si(100)2° surface is employed here for further low-defect III-V growth. After the Si surface preparation, a common approach is to subsequently grow a thin GaP nucleation layer, since this material is almost lattice matched to Si[1]. Here we apply AlxGa1-xP nucleation layer instead of established GaP-on-Si nucleation in order to further modify the atomic and electronic structure of the heterointerface as well as to yield adequate nucleation conditions. Prior to the nucleation, the Si(100)2° surface is exposed to TBAs in an Al-containing III-V MOVPE reactor. We observe that the oxide removal of the Si substrate by HF pre-treatment lowers the maximum process temperature below 820°C[2]. Subsequently the pulsed AlxGa1-xP nucleation layer consisting of Al, Ga, and P pulses is grown at 420°C, followed by a GaP epilayer growth at 600°C. The RAS signal of the grown GaP is benchmarked by low energy electron diffraction(LEED) and the surface morphology is studied by atomic force microscopy(AFM).[1]O. Supplie et al.,APL Mater.3(2015)126110.[2]A. Paszuk,...M. Nandy et al.,Sol. Energ. Mat. Sol. Cells,in press(2017),doi:10.1016/j.solmat.2017.07.032.

O 34: Plasmonics and nanooptics: Light-matter interaction, spectroscopy III

Time: Tuesday 14:00–15:30 Location: MA 041

O 34.1 Tue 14:00 MA 041

Towards near-field coupling of surface plasmon polaritons across sub-micrometer gaps — •Vladimir Smirnov, Sven Stephan, Heiko Kollmann, Jue-Min Yi, Christoph Lienau, and Martin Silies — Institute of Physics and Center of Interface Science, Carl von Ossietzky Universität Oldenburg, Germany

Efficient nanofocusing of light is one of the major tasks for the realization of an ultrafast, all-optical switch. For this purpose, Surface Plasmon Polaritons (SPP) need to be confined in a conical metallic stripe-like antenna to nm-dimensions using a curved grating coupler with a second conical antenna at a nanometer distance acting as a receiver.

Here, we study the propagation of SPPs using far-field confocal microscopy in a 200 nm thin Au film in a tapered waveguide geometry across gaps of down to 15 nm that are fabricated using the Focused Ion Beam-based "Sketch and Peel" technique [1]. For gap sizes smaller than 30 nm, the transmitted intensity abruptly increases indicating an enhanced energy transport through near-field coupling [2], in accordance with finite difference time domain calculations. Results of the present work are of interest in the field of efficient strong coupling of plasmons and excitons towards ultrafast optical switching.

[1] Y. Chen, et al., ACS Nano 10(12), pp 11228-11236 (2016)

[2] H. Kollmann, et al., Nano Lett 14(2), pp 4778-4784 (2014)

O 34.2 Tue 14:15 MA 041

Electron dynamics in gold nanotips — •Andreas Wöste, Thomas Quenzel, Jan Vogelsang, Petra Gross, and Christoph Lienau — Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany

Interaction between electrons and strong electromagnetic fields in solids plays a role in various physical phenomena, for example in optically induced emission of ultrashort electron pulses from metal nanotips. Besides the parameters of the incident laser pulses the electronic configuration of the emitter influences the emission process. On thin films, the electron dynamics are already intensely studied, mostly using two-photon emission pump-probe schemes. More recently, the electron dynamics in metal nanostructures come into focus, due to their potential as laser-triggered emitters in ultrafast electron microscopes. Unfortunately, the two-photon excitation schemes used typically cannot directly be transferred to nanostructures, because the need for wavelengths in the visible or UV regime often damages the samples. Therefore we show a measurement of electron relaxation times on chemicaly etched gold nanotips using multiphoton photoemission in a pump probe scheme with sub 20 fs laser pulses at center wavelengths of 600 nm and 1700 nm. We observe a four-fold increase of electron emission with respect to far delayed pulses, which indicates favored emission out of highly excited, non-thermal states which last for about 100 fs before they decay. The good agreement between our numerical model and the comparable timescale, in comparison with results from measurements on thin films, supports this suggestion.

O 34.3 Tue 14:30 MA 041

Vectorial near-field coupling — •Martin Esmann[1,2], Simon F. Becker[2], Julia Witt[2], Ralf Vogelgesang[2], Gunther Wittstock[2], and Christoph Lienau[2] — [1]CNRS Centre de Nanosciences et de Nanotechnologies (C2N), 91460 Marcoussis, France — [2]Carl von Ossietzky University, 26111 Oldenburg, Germany

The coherent exchange of optical near fields between two neighboring dipoles plays an essential role for the optical properties, quantum dynamics and thus for the function of many naturally occurring and artificial nanosystems[1,2]. These interactions are inherently short-ranged, extending over a few nanometers only, and depend sensitively on relative orientation, detuning and dephasing, i.e., on the vectorial properties of the coupled dipolar near fields. This makes it challenging to analyze them experimentally.

Here, we introduce plasmonic nanofocusing[3] spectroscopy to record coherent light scattering spectra with 5-nm spatial resolution from a small dipole antenna, excited solely by evanescent fields and coupled to plasmon resonances in a single gold nanorod. We resolve mode couplings, resonance energy shifts and Purcell effects as a function of dipole distance and relative orientation, and show how they arise from different vectorial components of the interacting optical near-fields. Our results pave the way for using dipolar alignment to control the optical properties and function of nanoscale systems.

[1] Zhang, Y. et al., Nature 531, 623 (2016).

[2] Scholes, G.D., et al., Nature Chemistry 3, 763 (2011).

[3] Stockman, M.I., PRL 93, 137404 (2004).

O 34.4 Tue 14:45 MA 041

Phase-resolved mapping of local optical near-fields around a single plasmonic nanoresonator — Martin Esmann, •Abbas Chimeh, Simon F. Becker, and Christoph Lienau — Institüt für Physik, Unversität Oldenburg

Plasmonic nanoantennas confine electromagnetic fields into nanoscale volumes. To fully understand and exploit this field localization, e.g., for nanoscale energy transport or for enhancing local nonlinear optical properties, a knowledge of their local optical response function, characterizing the electromagnetic fields emitted by the antenna in response to a point-like excitation in space and time, is highly desirable. Here, we show how to measure this local response function with ultrahigh, 5-nm spatial resolution by means of an isolated light spot, created by plasmonic nanofocusing [1]. Spectrally broadband surface plasmon polariton (SPP) waves are grating-coupled onto the shaft of conical gold taper and propagated towards the taper apex. The nanolocalized field at the apex locally excites a small gold rod acting as nanoantenna. The electric fields emitted by the rod are collected by the taper and emitted into the far field at a point scatterer at few microns distance from the apex. Its interference with a fraction of the incident light results in a spectral interferogram which carries full information on the local response of the antenna. By scanning the rod relative to the taper apex, we achieve fully spatially imaging of the local response function, directly mapping the dynamics of the locally emitted optical near field. [1] S. Schmidt et al., ACS Nano 6, 6040 (2012).

O 34.5 Tue 15:00 MA 041

Spectral shift and spectral broadening of broadband surface plasmon polaritons monitored in real-time during propagation — •Malte Grossmann[1], Paul Bittorf[1], Alwin Klick[1], Arkadiusz J. Goszczak[2], Jacek Fiutowski[2], Horst-Günter Rubahn[2], and Michael Bauer[1] — [1]Institute for Experimental and Applied Physics, University of Kiel, Kiel, Germany — [2]Mads Clausen Institute, NanoSYD, University of Southern Denmark, Sonderborg, Denmark

Interferometric time-resolved two-photon photoemission electron microscopy in a normal incidence configuration is used to monitor changes in the spectral distribution of a near-infrared broadband surface plasmon polariton (SPP) pulse as it propagates within 120 fs along a gold-vacuum interface. Next to a red-shift in the central frequency of the SPP pulse clear indications of spectral broadening are observed. The data are interpreted in terms of dispersive plasmon damping as qualitatively confirmed by numerical modeling of SPP propagation along a rough gold surface under consideration of ohmic losses and radiation damping.

O 34.6 Tue 15:15 MA 041

Exciton interaction with surface plasmon polaritons in hybrid metal-semiconductor nanostructures — •Felix Spitzer[1], Alexander N. Poddubny[2,3], Ilya A. Akimov[1,2], Victor F. Sapega[2], Lars Klompmaker[1], Lars E. Kreilkamp[1], Leonid V. Litvin[4], Ralf Jede[4], Grzegorz Karczewski[5], Maciej Wiater[5], Tomasz Wojtowicz[5,6], Dmitri R. Yakovlev[1,2], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]ITMO University, 197101 St. Petersburg, Russia — [4]Raith GmbH, Konrad-Adenauer-Allee 8, 44263 Dortmund, Germany — [5]Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland — [6]International Research Centre MagTop, PL-02668 Warsaw, Poland

We study the photoluminescence of diluted magnetic semiconductor CdMnTe/CdMgTe quantum well (QW) structures at low temperatures of 10 K using a Fourier imaging spectroscopy setup. It allows to observe the emitted lights intensity both angular and energy resolved. We demonstrate the coupling of QW exciton emission to surface plasmon polaritons close to the interface by observing a magnetic field induced change in emitted intensity. The effect decreases with increasing QW to surface distance.

O 35: Organic-inorganic hybrid systems and organic films IV

Time: Tuesday 14:00–15:45 Location: MA 042

O 35.1 Tue 14:00 MA 042

The role of Anchoring groups on Ruthenium (II) Bipyridine sensitized p-type semiconducor solar cells: A Quantum Chemical Calculation — •Anik Sen[1], Stephan Kupfer[2], Stefanie Grafe[2], and Axel Gross[1] — [1]Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany — [2]Institute for Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University Jena, D-07743 Jena, Germany

Ru (II) bipyridine complexes connected with p-type inorganic semiconductors (p-SC) such as NiO are promising systems for photocatalytic applications such as in dye sensitized solar cells (DSSC). The working principle is based on hole injection into the valence band of the p-type semiconductor from the photo excited semiconductor. We have performed both density functional theory (DFT) and time Dependent DFT calculations in order to understand the influence of different anchoring groups and spacer molecules attached to a photoactive Ruthenium bipyridine complex. The conversion efficiency of the dye molecules is predicted through our calculation. A model calculation of the anchors with the NiO surface is also calculated with the cluster approach, and implicit solvent model calculations are performed to understand the influence of the liquid environment.

In our discussion, we will try to shed light on the promising anchoring groups for the photocatalytic applications for p-SC.

O 35.2 Tue 14:15 MA 042

Theory of the geometry-dependent excitation transfer across a semiconductor/molecule interface — •Judith Specht[1], Björn Bieniek[2], Patrick Rinke[2,3], Andreas Knorr[1], and Marten Richter[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Aalto University, Aalto, Finland

Förster-type non-radiative coupling can transfer electronic excitations from inorganic semiconductor substrates to Frenkel excitons in organic molecular films. We analyze the excitation transfer efficiency as a function of the molecular geometry and other parameters such as charge carrier densities and temperatures.

Using a density-matrix equation technique, we study the case of creating excitons in an optically active layer of ladder-type quarterphenyl (L4P) molecules by strong electrical pumping of the electron-hole continuum in a ZnO quantum well substrate. Ab initio calculations provide the microscopic input parameters for our density-matrix equation technique [1,2]. Our findings reveal that the coupling efficiency strongly depends on multiple, but tunable parameters such as resonance energy detuning, molecular coverage, charge carrier occupation in the semiconductor substrate, distance between the constituents, and spatial orientation of the flat-lying molecules on the substrate. Our parameter study enables us to explore the operating regimes for optimized device performance.

[1] Verdenhalven et al., Phys. Rev. B 89, 235314 (2014).

[2] Specht et al., arXiv:1711.08955.

O 35.3 Tue 14:30 MA 042

Predictive first-principles modeling of complex inorganic/organic interfaces: PTCDA on Au(111) — •Victor G. Ruiz[1,2] and Alexandre Tkatchenko[1] — [1]Fritz-Haber Institut der MPG, Theory Department, Berlin, Germany — [2]Current affiliation: Helmholtz-Zentrum Berlin, Berlin, Germany

Understanding the properties of hybrid inorganic/organic systems has implications in both fundamental science and technology. An ab-initio modeling of these interfaces require efficient electronic-structure methods that capture accurately covalent and non-covalent interactions plus an atomistic model that includes complex adsorption configurations and an accurate surface representation. We present a predictive characterization of the structure and stability of perylenetetracarboxylic dianhydride (PTCDA) adsorbed on Au(111) within density-functional theory. Our calculations include collective many-body effects in the modeling of non-covalent interactions and a quantification of the self-interaction error in the adsorption energy of the system. We address effects due to single molecule/monolayer surface coverage and the role of the experimentally observed $22 \times \sqrt{3}$ surface reconstruction. Our approach yields an adsorption geometry in agreement with experiments within 0.1 Å and explains a difference of approximately 0.5 eV in the adsorption energy of the system which is observed when comparing atomic-force microscope and temperature-programmed desorption experiments. Our work shows that the inclusion of all relevant collective effects yields predictive power in the first-principles simulation of complex interfaces.

O 35.4 Tue 14:45 MA 042

Energy shift of the Ag (111) Shockley state due to adsorption of NTCDA — •Lukas Eschmann, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Molecular adsorption causes interaction between the electronic structure of adsorbate and substrate. One particular case is the energy shift of the Shockley surface state on Ag(111) and other surfaces: upon adsorption of organic molecules the state turns into an interface state and is shifted towards higher energy by as much as ~ 0.5 eV.

Here we address the interface state between the Ag(111) surface and adsorbed NTCDA within density-functional theory (DFT). To identify the interface state we have developed a projection technique which maps the states of the adsorbate system onto the original Shockley state. The projection also handles the loss of the surface periodicity due to the adsorbate, thus recovering the parabolic dispersion of the interface state in its original periodicity. We find that the energy shift of the Shockley state, as well as changes of its effective mass, are proportional to the adsorption coverage.

O 35.5 Tue 15:00 MA 042

Orbital Imaging of Non-Planar Molecules Beyond the Free Electron Finalstate Approximation — •Christian Metzger, Manuel Grimm, Martin Graus, Achim Schöll, and Friedrich Reinert — Julius-Maximilians-Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg, Germany

It has been shown that the imaging of molecular orbitals is possible by angle-resolved photoelectron spectroscopy (ARPES). For planar aromatic molecules the approximation of the photoemission final state by a simple plane wave allows for a particularly straightforward interpretation of the experimental data. Here we present a combined experimental and theoretical study on the angular intensity distribution of photoelectrons from non-planar molecules. The ARPES data of a single layer of C60 on Ag(110) was acquired by a momentum microscope which enables the efficient detection of photoelectrons emitted into the entire hemisphere above the sample. The symmetry of the recorded photoelectron momentum maps (PMM) immediately demonstrates that the molecules adsorb with a single specific alignment and do not rotate even at room temperature. On the theoretical side, a simple plane-wave approximation of the finalstate is bound to fail due to the 3D geometry of C60. A more suitable description can be realized within the framework of independent atomic centers (IAC), where the finalstate can be assembled by the composite contributions of the individual atoms inside the molecule. We demonstrate that this IAC approach provides a very good simulation of the experimental PMM and thus allows the assignment of different initialstate orbitals.

O 35.6 Tue 15:15 MA 042

Influence of Molecule Size on Surface Polymorph Formation — •Andreas Jeindl, Michael Scherbela, Lukas Hörmann, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Austria

Many properties of thin films, such as solubility or conductivity, are determined by the polymorph they assume upon adsorption on the (metal) substrate. In order to engineer functional interfaces, it is therefore imperative to understand and predict which polymorphs form for a given material combination. Yet, there are surprisingly few systematic studies that allow to deduct authoritative relationships between the molecular structure and the interface polymorph that will form. Computational studies are hindered by the intractably vast number of possible polymorphs, also known as 'configurational explosion'.

In this talk, we systematically investigate the influence of molecule size on the formation of surface polymorphs on the example of acenequinones on Ag(111). We present the SAMPLE approach that combines a physically motivated coarse-graining of the potential energy surface with machine learning as a method to overcome the configurational explosion. Precomputing the electrostatic and van-der-Waals interaction between adsorbate molecules allows us to extend the applicability of the method from model systems to technologically relevant molecules, such as acenequinones. For this example, we discuss the impact of the molecule size on the relative energies of selected polymorphs and the propensity to form low-energy defects.

O 35.7 Tue 15:30 MA 042

Rectification in molecular charge transfer systems — •Simon Liebing, Torsten Hahn, and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany

Charge transfer enabling rectification in molecular junctions was suggested by Ratner in 1974.[1] In the early 2000's strongly coupled system were excluded, because the strong coupling leads to symmetric transport behavior.[2] That left only weakly coupled charge transfer systems as candidates.[3] The authors studied different weakly coupling charge transfer dimers combining polycylic hydrocarbons and TNCQ-derivatives between gold leads. The observed rectifications are comparable to molecular systems using an asymmetric coupling to metallic leads. This shows that charge transfer is not alone suffient to achieve rectification in molecular electronics systems.

[1] Aviram, A. & Ratner, M. Chem. Phys. Lett. 29, 277 (1974)
[2] Mujica, V., Ratner, M. & Nitzan A. Chem. Phys. 281, 147 (2002)
[3] Hahn T., Liebing S., & Kortus J. Nanoscale 6, 14508 (2014)

O 36: 2D materials beyond graphene: TMDCs, silicene and relatives I

Time: Tuesday 14:00–16:00 Location: MA 043

O 36.1 Tue 14:00 MA 043

Tuning the electronic and magnetic properties of monolayer phosphorene by doping and strain — •Juliana Morbec[1], Gul Rahman[2], and Peter Kratzer[1] — [1]Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Physics, Quaid-i-Azam University, 45320 Islamabad, Pakistan

Phosphorene is an intriguing two-dimensional material with potential for a variety of applications. Its anisotropic optical and electronic properties combined with high carrier mobilities have attracted increasing attention in the past few years. Moreover, its superior mechanical flexibility has opened the possibility of tuning its electronic and magnetic properties by applying strain. Using first-principles calculations we investigate the interplay between defects, doping and strain on the electronic and magnetic properties of monolayer phosphorene. We find that (i) compressive strain can reduce the band gap of pristine phosphorene and induce a semiconductor-to-metal transition; and (ii) tensile strain can reduce the formation energy of magnetic single vacancies and lead to the stabilization of these defects. Our results also show that carbon-doping induces magnetism and a semiconductor-to-metallic transition; compressive biaxial strain has been found to suppress the magnetism whereas tensile strain opens the band gap and leads to an increase in the magnetic moment. Our findings suggest that doping and applying strain are important methods to tune the electronic and magnetic properties of monolayer phosphorene.

O 36.2 Tue 14:15 MA 043

An electrically controlled single atom magnetic switch on black phosphorus — •Brian Kiraly, Werner v. Weerdenburg, Alexander N. Rudenko, Mikhail I. Katsnelson, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

Single atoms at the surfaces of solids have demonstrated rich electronic, chemical, and magnetic properties. In this direction, we demonstrate that we can manipulate the orbital population of a single cobalt atom on a crystalline black phosphorus surface. Using the local electric field generated from an STM tip, individual cobalt atoms residing at the same hollow site can be reversibly switched between two stable states, which correspond to the different orbital configurations. The experimentally observed charge density of each configuration is corroborated with density functional theory calculations, which reveal the total magnetic moment and relaxation of the cobalt atom, as well as the electronic properties of the cobalt atom which locally dopes the black phosphorus. Utilizing tip-induced band bending, we further study the screening behavior of each Co atom configuration. We investigate the stability of each configuration, as well as compare the experimentally measured impurity states with DFT calculations. This system provides a new perspective on the horizon for fundamental properties of single atoms on surfaces.

O 36.3 Tue 14:30 MA 043

Characterisation of Defects in black phosphorus and phosphorene — •Julian Gaberle[1], Alexander Shluger[1], Mark Wentik[1], Tony Kenyon[1], and Alexander Schwarz[2] — [1]University College London, WC1E 6BT London, UK — [2]University of Hamburg, 20355 Hamburg, Germany

Interest in black phosphorus as a post graphene material has attracted considerable attention since 2014. Similar to graphene it consists of vdW bonded layers of covalently bonded phosphorus atoms. However, unlike graphene BP has a tunable direct bandgap, displays very high hole mobility and current switching ratios, which make it an interesting candidate for modern technologies.However, in order to make the transition from research labs to modern technologies the fundamental properties of BP and phosphorene need to be better understood. In particular point defects in the lattice and their effect on the electronic properties of BP are still not fully understood.

To characterise these defects, STM imaging was performed on black phosphorus and extended anisotropic defect states were observed. These defects have previously been attributed to phosphorus vacancies, but recently it has been suggested that Sn impurities are an alternative defect source. In oder to better understand the nature of the defect, atomically resolved AFM imaging and XPS was performed. Combining state of the art experiments with ab initio DFT modelling of vacancies and impurities, we were able to eliminate Sn impurities as a likely source of these defects and propose that these are indeed vacancies created in the cleavage process.

O 36.4 Tue 14:45 MA 043

Engineering Kondo State in Two-Dimensional Semiconducting Phosphorene — •Rohit Babar[1] and Mukul Kabir[1,2] — [1]Department of Physics, Indian Institute of Science Education and Research, Pune, India — [2]Center for Energy Science, Indian Institute of Science Education and Research, Pune, India

Correlated interaction between dilute localized electrons with the itinerant conduction electrons gives rise to Kondo effect below sufficiently low temperature. Beyond the conventional impurity in a metal systems, many artificial Kondo systems have been discovered in the last two decades. In sharp contrast to the artificial Kondo systems, we report an intrinsic, robust and high-temperature Kondo state in two-dimensional semiconducting phosphorene based on density functional theory calculations at different levels of approximations. While absorbed at a thermodynamically stable lattice defect, Cr impurity triggers an electronic phase transition in phosphorene to provide conduction electrons, which strongly interact with the localized moment generated at the Cr site. This manifests in an intrinsic Kondo state, where a multi-stage quenching of the impurity moment occurs in the temperature range 40-200 K. Further, along with a significantly small extension of Kondo cloud, the predicted Kondo state is shown to be robust under uniaxial strain and layer thickness, which greatly simplifies its future experimental realization. Our findings will broaden the current understanding of Kondo physics in two-dimensional materials.

O 36.5 Tue 15:00 MA 043

Investigating mechanical-high order elastic constants- and electronic properties of single layer borophene — mahdi faghihnasiri[1], homayoun jafari[2], •mostafa shabani[1], and sina malakpour estalaki[3] — [1]department of physics, shahrood university of technology, shahrood, iran — [2]department of physics, iran university of science and technology, tehran, iran — [3]department of aerospace and mechanical engineering, university of notre dame, Indiana, usa

Very recently two-dimensional layers of boron atoms, so-called borophene, have been successfully synthesized on the silver surfaces and attracts tremendous interest.

Borophene exhibits various structural polymorphs all of which are metallic. In this work, under in-plane uniaxial/biaxial strain/stress, we employ first-principles density functional theory calculations to investigate the electronic and mechanical properties of three single-layer borophene sheets (β12, χ3, and striped borophene).

In the mechanical section, nonlinear in-plane elastic properties of borophene are calculated and we proposed a method to study high order elastic constants of the 2D rectangular structures. The continuum description of the elastic properties of monolayer borophene sheets is obtained using this method through ab initio density functional theory.

In electronic properties section by analyzing electronic band structure we observed an anisotropic behavior. Despite metallic character of borophene sheets, applying directional strain based on deformation matrices, create a band gap in some regions of Brillouin zones.

O 36.6 Tue 15:15 MA 043

Investigation of hexagonal boron-nitride (hBN) and graphene Gr-R0° on SiC(0001) — •Markus Franke[1,2], Shayan Parhizkar[1,2], Serguei Soubatch[1,2], You-Ron Lin[1,2], Nafiseh Samiseresht[1,2], Miriam Raths[1,2], Janina Felter[1,2], François C. Bocquet[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, 52425 Jülich, Germany

Among other 2D materials, hexagonal boron-nitride (hBN) seems to be a promising candidate for a new substrate material to achieve truly free-standing graphene layers. It forms a flat hexagonal lattice structure with a lattice parameter similar to that of graphene, but (in contrast to graphene) it is insulating (band gap $> 5\,\mathrm{eV}$). Here we report on the formation of hBN/SiC(0001) and on the subsequent preparation of graphene layers having the same orientation as the underlying SiC substrate (Gr-R0°). This orientation is unusual, typically epitaxial graphene on SiC(0001) is rotated by 30° (Gr-R30°).

We discuss the preparation of the layers performed by annealing SiC wafers in a borazine ($B_3N_3H_6$) atmosphere, and their properties based on results from core-level and angular resolved valence level electron spectroscopy (XPS and ARPES), as well as X-ray standing waves (XSW).

O 36.7 Tue 15:30 MA 043

Kelvin Probe Force Microscopy examination of defects of h-BN on Pt(111) — •Gino Günzburger, Roland Widmer, Liwei Liu, and Oliver Gröning — Nanotech@surfaces Laboratory, Empa - Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

Epitaxial hexagonal boron nitride (h-BN) is an interesting material, which has attracted significant scientific interest for more than a decade. It has a hexagonal structure similar to the one of Graphene and it forms monolayers on many metals. The mono-layers have varying and interesting structures, such as a flat and even layers as on Ni(111), specific Moiré-patterns such as on Pt(111) and corrugated structures called "nanomesh" due to their mesh-like appearance (e.g on Rh(111)). The structure of the formed layer depends not only on the lattice mismatch between the h-BN and the substrate, but also on the strength of the interaction between the two [1]. We deposited an h-BN monolayer on Pt(111) by thermal decomposition of borazine (Cyclotriborazan, (BHNH)3) on the hot substrate and subsequently examined it by STM and Kelvin Probe Force Microscopy (KPFM) using a Qplus STM/AFM in UHV at approximately 5K. On Pt(111) h-BN forms a Moiré pattern showing bright dots on a darker background when examined by STM at a high gap voltage. Defects in the h-BN appear as black spots in the STM image. They were located by STM, examined by KPFM and identified as regions of higher work function.

[1] L. Camilli, E. Sutter and P. Sutter, 2D Materials 1, 025003 (2014)

O 36.8 Tue 15:45 MA 043

Corrugation in the weakly interacting *h*-BN/Cu(111) system — Martin Schwarz[1], Alexander Riss[1], Manuela Garnica[1], Jacob Ducke[1], Peter S Deimel[2], David A Duncan[2], Pardeep Kumar Thakur[2], Tien-Lin Lee[2], •Ari P Seitsonen[3], Johannes V Barth[1], Francesco Allegretti[1], and Willi Auwärter[1] — [1]Technical University of Munich, Department of Physics, Garching — [2]Diamond Light Source, Harwell Science and Innovation Campus, Didcot — [3]Département de Chimie, École Normale Supérieure, Paris

Atomically thin hexagonal boron nitride (*h*-BN) layers on metallic supports represent a promising platform for the selective adsorption of atoms, clusters, and molecular nanostructures. Here we employ complementary techniques including high-resolution noncontact atomic force microscopy, scanning tunnelling microscopy, low-energy electron diffraction, X-ray photoelectron spectroscopy, the X-ray standing wave method, and density functional theory to yield a comprehensive, quantitative structure determination including the adsorption height and the corrugation of the sp^2-bonded *h*-BN layer on Cu(111) [1]. We compare the results to the adsorption structures of *h*-BN on other transition and coinage metal surfaces, in particular to *h*-BN/Ir(111) [2,3].

[1] Schwarz *et alia*, ACS Nano **11**, 9151-9161 (2017); DOI: 10.1021/acsnano.7b04022

[2] zum Hagen *et alia*, ACS Nano **10**, 11012-11026 (2016); DOI: 10.1021/acsnano.6b05819

[3] Seitsonen, Schulz and Liljeroth, in preparation

O 37: Electronic-Structure Theory: General II

Time: Tuesday 14:00–16:15 Location: MA 141

Invited Talk O 37.1 Tue 14:00 MA 141

Unraveling the structure and dynamics at solid-liquid interfaces by machine learning potentials — Matti Hellström[1], Vanessa Quaranta[2], and •Jörg Behler[1] — [1]Theoretische Chemie, Universität Göttingen, Germany — [2]Theoretische Chemie, Ruhr-Universität Bochum, Germany

Solid-liquid interfaces pose a significant challenge for atomistic simulations. The very different interactions and bonding situations in water and in solid surfaces are best described by electronic structure methods, which can also take into account the dissociation and recombination of water molecules at the interface. On the other hand, long simulations of large systems are required to obtain converged properties of the liquid phase, which is often computationally very demanding. Machine learning potentials offer a solution to this problem by combining a first principles quality description of the potential-energy surface with the efficiency of simple empirical potentials. In this talk, recent results for the interaction of water with metal and oxide surfaces will be presented, which have been obtained in molecular dynamics simulations employing high-dimensional neural network potentials (NNPs), a typical class of machine learning potentials. NNPs are reactive and thus allow to observe proton transfer processes at the interface, which also play an important role in highly concentrated electrolyte solutions.

O 37.2 Tue 14:30 MA 141

Representing energy landscapes by combining neural networks and the empirical valence bond method — •Sinja Klees[1], Eckhard Spohr[2], and Jörg Behler[1,3] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, D-45141 Essen, Germany — [3]Theoretische Chemie, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany

Computer simulations of aqueous electrolyte solutions can be challenging for several reasons: (i) there can be huge variations in the ratio of solvent molecules and ions; (ii) large-scale simulations are needed to avoid artificial periodicity and (iii) reactive potentials are necessary to take omnipresent proton transfer reactions into account. Artificial neural networks (NNs) are a powerful method to construct reliable and unbiased interatomic potentials for a wide range of 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. Combining NN potentials of different system fragments with the empirical valence bond (EVB) method offers a promising approach to derive the potential energy surface of complex systems with substantially reduced effort. Preliminary results will be discussed and compared to density functional theory data.

O 37.3 Tue 14:45 MA 141

Ultra long-range ab-initio calculations — •Tristan Müller[1],

Sangeeta Sharma[1,2], Eberhard K.U. Gross[1], and John K. Dewhurst[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germay — [2]Department of Physics, Indian Institute of Technology-Roorkee, 247667 Uttarakhand, India

We propose a generalization of the Bloch state which involves an additional sum over a finer grid in reciprocal space around each k-point. This allows for ab-initio calculations of ultra long-range modulations in the density which may involve millions of unit cells but with an efficiency rivaling that of a single unit cell. Thus physical effects on the micron length scale, which nevertheless depend on details of the electronic structure can be computed exactly within density functional theory. As an example, we apply our method to solids subjected to spatially extended external electromagnetic fields.

15 min. break

O 37.4 Tue 15:15 MA 141

Optical Spectra from TDDFT with an Adiabatic GGA XC Kernel — •Nisha Singh[1,2], Peter Elliott[1], J.K. Dewhurst[1], E.K.U. Gross[1], and Sangeeta Sharma[1,2] — [1]Max-Planck Institute of Microstructure Physics, Halle, Germany — [2]Indian Institute of Technology Roorkee, Roorkee, India

A complete understanding of a material requires both knowledge of the excited states, as well as the ground state. Time dependent density functional theory (TDDFT), within the linear response regime, has been a successful method to access these excited state properties. However, it suffers the drawback that the exchange-correlation (XC) kernel must be approximated. In this work, we climb up 'Jacob's ladder' of functionals and use a adiabatic generalized gradient approximation (AGGA) for the XC kernel, rather than the commonly used adiabatic local density approximation (ALDA). The performance of the AGGA kernel is assessed for simple solids by studying optical absorption spectra. We find better results, as compared to the ALDA kernel, when gradients of density are included in the XC kernel.

O 37.5 Tue 15:30 MA 141

First Principles Simulations of Small Polarons in Ionic Crystals — •Maria Dragoumi, Sebastian Kokott, Sergey Levchenco, Igor Ying Zhang, and Matthias Scheffler — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

A small polaron can be modeled by a supercell with a hole or an electron in periodic boundary conditions. In order to correctly cover long-range contribution, very large supercells are often needed, which makes advanced first principles simulations prohibitively expensive to run. In this work, we propose a force-field corrected model to efficiently describe the lattice distortion due to the long range contribution in a reasonably small supercell model [1]. In this approach the electronic structure close to the center is treated accurately, on the theoretical levels of semilocal PBE, hybrid HSE06, and second-order Møller-Plesset perturbation theory, but taking into account the contribution of elastic distortion of the distant atoms by an appropriate model hamiltonian. The convergence behavior of long-range contribution in this hybrid strategy is examined and we apply this method to study the geometry distortion of the small polaron in MgO. The results are compared to other calculations using standard supercell models and to available experimental data.

[1] M. Scheffler, J.P. Vigneron, and G. B. Bachlelet, Phys. Rev. B 31, 6541 (1985).

[2] S. Kokott, S. V Levchenko, P. Rincke, and M. Scheffler, Submitted, arxiv:1710.03722 (2017).

O 37.6 Tue 15:45 MA 141

Vibrational Anharmonic Raman Spectra of Polymorphic Crystals from Density-Functional-Perturbation Theory — •Nathaniel Raimbault, Honghui Shang, and Mariana Rossi — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Vibrational Raman spectroscopy is widely used for characterizing different molecular-crystal polymorphs and their phase transitions. Few theoretical studies take anharmonic effects into account, despite their acknowledged importance in particular in organic and flexible compounds. In this work we compute anharmonic Raman spectra through the calculation of polarizability autocorrelation functions in thermodynamic equilibrium, obtaining polarizability tensors from our recent implementation of Density Functional Perturbation Theory (DFPT) in the all-electron FHI-aims code [1,2]. We focus here on different polymorphic forms of the paracetamol and aspirin crystals. Our anharmonic calculations show important effects in the low-frequency range of these spectra which prove essential for obtaining agreement with experimental data. Furthermore, in order to reduce the cost of DFPT simulations we use Kernel Ridge Regression (KRR) to obtain DFPT-level polarizabilities at a reduced cost. Training our model on a few thousand points, we can reproduce Raman spectra that would typically take the calculation of hundreds of thousands of points. [1] H. Shang *et al.*, CPC **215**, 26 (2017) [2] H. Shang, N. Raimbault, *et al.*, submitted (2017)

O 37.7 Tue 16:00 MA 141

Engineering one-body density-matrix functionals — •Carlos L. Benavides-Riveros[1], Nektarios Lathiotakis[2], and Miguel A. L. Marques[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, GR-11635 Athens, Greece

The problem of computing ground states of systems of many electrons is at the very heart of many-body quantum physics. This problem is so challenging that a major goal in electronic modelling is to reduce that hardness much more below the one of the wave function. Density and reduced-density-matrix functional theories achieve a maximal reduction by using, respectively, the electronic density and the one-body reduced density matrix (1RDM) as the basic variables. In the literature there are several functionals of the 1RDM for closed shell systems. Based on recent progress on fermionic exchange symmetry, we produce a family of functionals for systems with odd numbers of active electrons. Since the general structure of the functionals is derived from general pure representability considerations, our approach suggests a systematic way to produce functionals within reduced density matrix functional theory.

O 38: Metal substrates: Adsorption of atoms and inorganic molecules

Time: Tuesday 14:00–15:45 Location: MA 144

O 38.1 Tue 14:00 MA 144

Controlling the competition between Kondo effect and spin-orbit interaction in a single molecule by atomic manipulation — •Emi Minamitani[1], Ryoichi Hiraoka[2], Ryuichi Arafune[3], Noriyuki Tsukahara[2], Satoshi Watanabe[1], Maki Kawai[2], and Noriaki Takagi[2] — [1]Department of Materials Engineering, The University of Tokyo — [2]Department of Advanced Materials Science, The University of Tokyo — [3]WPI-MANA, National Institute for Materials Science,

Magnetic molecules on metal surfaces are good playground to investigate and control the magnetic properties of nanostructures. In these systems, the Kondo effect and spin-orbit interaction (SOI) are two major components to determine the magnetism. When the molecule has an integer spin, these components compete each other. If the Kondo effect dominates over the SOI, the Kondo singlet state appears. On the other hand, the zero-field splitting spin state appears in the SOI dominant case. Here we report the control of the transition between these two states in iron phthalocyanine (FePc) on Au(111) by molecular manipulation with scanning tunneling microscope (STM) and elucidate the mechanism by the density functional theory (DFT) and numerical renormalization group (NRG)[1].

[1] R. Hiraoka, E. Minamitani, R. Arafune, N. Tsukahara, S. Watanabe, M. Kawai, N. Takagi, Nat. Commun 8 16012 (2017).

O 38.2 Tue 14:15 MA 144

First-Principles Compressed-Sensing Study of Oxygen Adsorption at Transition-Metal Surfaces — Somayeh Faraji[1,2], •Sergey V. Levchenko[1], Runhai Ouyang[1], Luca M. Ghiringhelli[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin 14195, Germany — [2]Faradayweg 4-6

Understanding the interaction of transition metals (TMs) and alloys with reactive species such as oxygen is important for the design of new catalysts [1]. We use density-functional theory calculations combined with compressed sensing to identify descriptors for adsorption energy of O atom at flat and stepped TM surfaces. The RPBE functional [2] is chosen based on its performance in comparison to available experimental results. Using sure independence screening with the l_0 sparsifying operator (SISSO) [3], we identify physically interpretable descriptors that predict O adsorption energies based solely on properties of involved species, bulk, and clean surfaces. The maximum absolute error of the prediction is within 0.25 eV. The identified descriptor is built from the following contributions describing the strength of the surface-O interaction: i) surface energy, ii) number of valence electrons in the metal atom, iii) *d*-band center, iv) difference between the work function and O ionization energy, and v) difference between the *d*-band center and the *s*-level of the metal atom.

[1] A. Vojvodic and J. K. Nørskov, National Sci. Rev. **2**, 140 (2015)
[2] B. Hammer *et al.*, Phys. Rev. B **59**, 7413 (1999)
[3] R. Ouyang *et al.*, arXiv:1710.03319 (2017)

O 38.3 Tue 14:30 MA 144

Interaction process of a CO molecule on a copper surface with a metallic tip of a microscope — •Norio Okabayashi[1,2], Angelo Peronio[2], Daniel Meuer[2], Sonia Matencio[2], Ferdinand Huber[2], Magnus Paulsson[3], Toyoko Arai[1], and Franz J. Giessibl[2] — [1]Kanazawa University, Kanazawa, Japan — [2]University of Regensburg, Regnsburg, Germany — [3]Linnaeus University, Kalmer, Sweden

In order to investigate the vibrational state of a CO molecule put in the force field by a metallic tip, we have developed a method combining atomic force microscopy and inelastic electron tunneling spectroscopy (IETS). In previous, we reported that considering the bond elongation is crucial to reproduce the vibrational energy shift in the force field as well as the linear superposition of the perturbed force. We also reported that the distance dependent IETS intensity can be interpreted by combining the concept of the bond elongation with our previous finding on the IETS intensity [1] that the intensity strongly depends on the fraction of the current passing through the molecule. Here we have improved our method by stabilizing the tip oscillation during the IETS measurements and extended the measurements to the smaller tip molecule distance for the system of a CO molecule on a Cu(111) surface. We demonstrate that the improved data provides the interpretation consistent with our previous conclusion along with the new insight into the tip molecule interaction process. [1] N. Okabayashi, A. Gustafsson, A. Peronio, M. Paulsson, T. Arai, and F. J. Giessibl, Phys. Rev. B 93, 165415 (2016).

O 38.4 Tue 14:45 MA 144

Control of rotational oscillation by protonation in single triazatruxene molecules — •Anja Bauer[1], Markus Maier[2], Werner Schosser[1], Philipp Erler[1], Florian Singer[1], Fabian Pauly[1], Yuriy Dedkov[3,1], Rainer Winter[2], and Mikhail Fonin[1] — [1]Department of Physics, University Konstanz, D-78457 Konstanz — [2]Department of Chemistry, University Konstanz, D-78457 Konstanz — [3]Department of Physics, Shanghai University, 200444 Shanghai, China

The opportunity of tuning the electric and magnetic properties [1] as well as the control of molecular motions on surfaces [2], [3], [4] is of great interest since it lays a foundation for the fabrication of molecule-based functional devices. Here we investigate the behavior of single triazatruxene (TAT) molecules on Ag(111) deposited by electrospray ionization method. Low temperature STM measurements reveal three different types of molecular appearance on Ag(111) which we assign to the non-, single- and double-protonated TAT. In non-protonated molecules tunneling current is shown to excite rotational oscillations between two stable adsorption configurations. Protonation, however, leads to an efficient suppression of the rotational oscillation and of the lateral mobility of the molecules. We further show the possibility to switch the oscillation on and off by detaching or attaching hydrogen to the nitrogen atoms of TAT.

[1] B. Borca et al., ACS Nano 9, 12506 (2015), [2] I. Swart et al., Nano Letters 12, 1070 (2012), [3] A. Krönlein et al, J. Phys. Chem. 120, 13843 (2016), [4] H.W. Kim et al., Phys. Rev. Lett. 106, 146101 (2011)

O 38.5 Tue 15:00 MA 144

Oxidation of Transition-Metal Surfaces: A Cluster-Expansion Study — •Zhong-Kang Han[1], Ray Miyazaki[3], Somayeh Farajinafchi[1], Santiago Rigamoni[2], Maria Troppenz[2], Jun-ya Hasegawa[3], Sergey V. Levchenko[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin 14195, Germany — [2]Humboldt–Universität zu Berlin, Berlin 12489, Germany — [3]Hokkaido University, Sapporo 001-0021, Japan

Oxidation of metal surfaces plays a fundamental role when functional devices are in contact with an oxidizing environment. The thermodynamics of oxidation and its dependence on the metal type and surface cut are still not fully understood. We study the adsorption of atomic oxygen at Au, Pt, Ni (110), and Rh (100) surfaces, using a cluster-expansion model, parametrized with RPBE calculations. We find that atomic oxygen randomly adsorbs on the short-bridge site of Au(110) or Pt(110) at low coverages (<25%), forming a $c(2\times2)$ pattern as the coverage increases. For coverage >25%, this pattern is destabilized, and a new pattern $c(2\times\sqrt{2})$ will form with top and hollow sites occupied. Interestingly, although O at short-bridge sites is most stable at low coverages, no short-bridge sites are occupied by oxygen at the coverage of 50%. On the contrary, Ni (110) passes through a variety of ordered adsorbed O phases as the coverage is increased, with a mixed occupation of the short-bridge and other sites. Increasing coverage above 75% for Pt (110) or Ni(110), and above 50% for Au(110) or Rh (100) leads to destabilization of dissociative versus molecular adsorption.

O 38.6 Tue 15:15 MA 144

Effect of polymer coating on H2 adsorption/desorption on Palladium nanoparticles — •Lucy Cusinato and Anders Hellman — Department of Physics, Chalmers University of Technology, Göteborg, Sweden

Palladium-based materials have been known for their capacity to form hydride phases, making them good candidates for hydrogen storage applications. These applications rely on two fundamental features of metallic palladium: the ability to dissolve hydrogen to form stable hydride and the possibility to easily release the stored hydrogen. Efforts have been made to improve the storage capacity and kinetics, either by modification of the metallic core or by varying the environment of the palladium material. Experimentally, the presence of metal-organic frameworks or polymers has been shown to improve the kinetics of hydrogen storage. Here, we study this phenomenon from a theoretical (using DFT) point of view in close collaboration with experimentalists. The behavior of palladium and palladium hydride nanoparticles towards H2 adsorption and desorption, with and without polymer (PTFE, PVDF and PMMA) coating, is studied. A particular focus is set on how to model this kind of nanoparticle/polymers systems for the case of bare and hydride palladium. Stability of palladium hydride nanoparticles is studied, as well as different types of interaction at the Pd-polymer interface. These results are then used to shed light on how the presence of polymers, and the existence of a palladium/polymer interface, can affect the kinetics and thermodynamics of the system in order to facilitate H2 adsorption and desorption processes.

O 38.7 Tue 15:30 MA 144

Ester formation without any catalyst at the liquid-solid interface — •Nguyen Thi Ngoc Ha[1], Gopakumar T. G.[2], Yen N. D. C.[1], Carola Mende[3], Lars Smykalla[1], Roy Buschbeck[3], Tobias Rüffer[3], Heinrich Lang[3], Maik Schlesinger[4], Michael Mehring[4], and Michaele Hietschold[1] — [1]Solid Surfaces Analysis Group, Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India — [3]Inorganic Chemistry, Institute of Chemistry, Technische Universität Chemnitz, Chemnitz, Germany, — [4]Coordination Chemistry, Institute of Chemistry, Technische Universität Chemnitz, Chemnitz, Germany

A chemical reaction (esterification) within a molecular monolayer induced by increasing the molecular packing density of this layer at a liquid-solid interface is studied by ambient scanning tunnelling microscopy (STM). The self-assembled ordered monolayer consisting of trimesic acid and undecanol/decanol with a molecular ratio of both species of 1:1 forms at the interface to the highly oriented pyrolytic graphite (HOPG) out of a solution of TMA in decanol/undecanol. As the packing denisty is increased at interface, by extended sonication, heating or stirring of the solution the trimesic acid reacts with undecanol/decanol within the monolayer and froms a monoester without the presence of any catalyst. The ester formation at the interface is further confirmed by theoretical calculations and chemical analysis of the solutions using different methods.

O 39: Focus Session: Phonon Polaritons: Opportunities for THz Nanooptics II

Time: Tuesday 14:00–15:30 Location: HE 101

O 39.1 Tue 14:00 HE 101

Highly-confined surface phonon polaritons in metal circular cavities fabricated on a phase change material — •Hisashi Sumikura[1,2], Andreas Hessler[1], Lena Jung[1], Martin Lewin[1], and Thomas Taubner[1] — [1]RWTH Aachen University, Aachen, Germany — [2]NTT Basic Research Laboratories, Atsugi, Japan

To enhance the interaction between light and nanomaterials, the light field should be concentrated into a small volume while overcoming the diffraction limit. In the mid-infrared region, surface phonon polaritons (SPhPs) confined in optical cavities show their strong field concentration. We have studied on metal circular cavities on SiC [1] and laser-induced dielectric cavities in a phase change material on quartz [2] to achieve SPhP confinement.

In this study, we demonstrate cavity-confined mid-infrared SPhPs in a thin film of germanium-antimonide-telluride (GST) deposited on SiC. Scattering-type scanning near-field optical microscopy showed that a 1-μm-diameter metal circular cavity achieves a strong field concentration of the SPhP with a width of less than 250 nm, that is 1/44 of the wavelength of incident light (11.1 μm). In addition, the thermal annealing of the samples switched the SPhP confinement off with a large detuning of the resonance, which is induced by the change in optical constants of phase-changed GST.

[1] T. Wang, P. Li, B. Hauer, D. N. Chigrin, T. Taubner. Nano Lett. 13, 5051 (2013). [2] P. Li, X. Yang, T. W. W. Mass, J. Hanss, M. Lewin, A-K. U. Michel, M. Wuttig, T. Taubner. Nature Mater. 15, 870 (2016).

O 39.2 Tue 14:15 HE 101

Strong Coupling of a Surface Phonon Polariton and an Epsilon Near Zero Mode — •Nikolai Christian Passler[1], Christopher Gubbin[2], Ilya Razdolski[1], Martin Wolf[1], Simone De Liberato[2], Joshua Caldwell[3], and Alexander Paarmann[1] — [1]Fritz-Haber-Institute of the MGP, Berlin,Germany — [2]University of Southampton, UK — [3]Vanderbilt University, Nashville, USA

Surface phonon polaritons (SPhP) supported in polar dielectrics constitute a promising route for the development of low-loss mid infrared (MIR) nanophotonics [1]. In sub-wavelength thin layers, ultrathin film polaritons arise at the longitudinal optical phonon frequency where the dielectric permittivity crosses zero. These intrinsic epsilon near zero (ENZ) polariton modes exhibit immense wavelengths, giving rise to remarkable phenomena like supercoupling or light trapping [2].

Employing an MIR free-electron laser and the Otto geometry for prism coupling [3], we here experimentally map out the dispersions of SPhPs in an ultrathin AlN layer on top of bulk SiC. Our measurements reveal strong coupling of the bulk SiC SPhP to the ENZ mode supported by the thin layer, resulting in ENZ SPhP modes which provide the promising possibility to incorporate ENZ wave propagation attributes into polaritonic nanophotonics.

[1] Caldwell et al., Nanophotonics 4, 44 (2015)

[2] Liberal et al., Nature Photonics 11, 149 (2017)

[3] Passler et al., ACS Photonics 4, 1048 (2017)

O 39.3 Tue 14:30 HE 101

Surface-Enhanced Terahertz Spectroscopy of Organic Molecules — •Lucca Kühner[1], Weiwu Li[2], Frank Neubrech[1,3], Martin Dressel[2], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart — [2]1st Physics Institute, University of Stuttgart — [3]Kirchhoff-Institute for Physics, University Heidelberg

Mid-infrared (MIR) spectroscopy allows for label-free identification of chemical species by their characteristic intramolecular vibrations and is thus widely used in biology, pharmacy, and medical sciences. For isomeric molecules, e.g., monosaccharides such as glucose and fructose which have the same chemical bonds and similar spatial arrangement, vibrational bands in the MIR region do mostly not provide sufficient specific information. In contrast, terahertz (THz) spectroscopy probes intermolecular interactions in mostly crystalline structures and is thus sensitive to the molecule's conformation. This technique is consequently able to differentiate between isomeric molecules. However, the absorption cross-section of such intermolecular interactions is even lower than for MIR spectroscopy. To overcome this limitation, we are going to extend the concept of surface-enhanced infrared spectroscopy (SEIRS) to the THz wavelength range. In this work, we demonstrate measurements of two crystalline configurations of Glucose in the THz region. By introducing surface-enhanced THz spectroscopy we aim at improved sensitivity.

O 39.4 Tue 14:45 HE 101

Phonon-Polaritonic Bowtie Nanoantennas: Controlling Infrared Thermal Radiation at the Nanoscale — Tao Wang[1], Peining Li[1], Dmitry N. Chigrin[1,2], Alexander J. Giles[3], Francesco J. Bezares[4], Orest J. Glemboki[3], Joshua D. Caldwell[3,5], and •Thomas Taubner[1] — [1]RWTH Aachen University, Aachen, Germany — [2]DWI Leibniz Institute for Interactive Materials, Aachen, Germany — [3]U.S. Naval Research Laboratory, Washington DC, USA — [4]Universidad de Puerto Rico, Cayey, Puerto Rico — [5]Vanderbilt University, Nashville, TN, USA

A conventional thermal emitter exhibits a broad emission spectrum with a peak wavelength depending upon the operation temperature. Narrowband thermal emission can be realized with periodic gratings or single microstructures hosting Surface Phonon-Polaritons (SPhPs) [1-3], offering lower losses and higher resonance quality factors than the commonly used Surface Plasmon Polaritons (SPPs). Here, we investigate the coupling of adjacent phonon-polaritonic nanostructures, specifically deeply sub-diffractional bowtie-shaped silicon carbide nanoantennas. We employ infrared far-field reflectance spectroscopy and compare it with full-wave electromagnetic simulations and near-field optical nanoimaging. We experimentally demonstrate that the nanometer-scale-gaps can control the thermal emission frequency while retaining emission linewidths as narrow as 10 cm-1[4].

[1] J. J. Greffet et al, Nature 416, 61 (2002). [2] J. A. Schuller et al, Nature Photon. 3, 658 (2009). [3] J. D. Caldwell, et al., Nanophotonics 4, 44 (2015). [4] T. Wang et al., ACS Photonics 4, 1753 (2017).

O 39.5 Tue 15:00 HE 101

Nonlinear nanophotonics with localised phonon polaritons — •Simone De Liberato and Christopher Gubbin — School of Physics and Astronomy, University of Southampton, Southampton, UK

Phonon polaritons localised in nanometric resonators are a promising platform to develop polaritonic applications in the terahertz and mid-infrared regions. This is due to their extremely small mode volumes, long lifetimes, and large nonlinearities; as well as the relative ease with which nanoresonators with features at the 100nm scale, are fabricated.

In this talk I will present our recent results in this field. I will start with the experimental demonstration of strong coupling between localised and propagative phonon polariton modes in SiC nanopillar arrays [1]. I will then review a series of theoretical works in which, by investigating nonlinear properties of localised phonon polaritons, we demonstrate the possibility to exploit them to empower a novel generation of terahertz and mid-infrared devices [2-4].

[1] C. R. Gubbin, F. Martini, A. Politi, S. A. Maier, and S. De Liberato, Phys. Rev. Lett. 116, 246402 (2016)

[2] C. R. Gubbin, S. A. Maier, and S. De Liberato, Phys. Rev. B 95, 035313 (2017)

[3] C. R. Gubbin and S. De Liberato, ACS Phot. 4, 1381 (2017)

[4] C. R. Gubbin and S. De Liberato, ACS Phot. 10.1021/acsphotonics.7b00863 (2017)

O 39.6 Tue 15:15 HE 101

Towards nanoscale time-domain-spectroscopy at low-repetition-rate terahertz sources — •Thales V. A. G. de Oliveira[1,2], Frederik Kuschewski[1], Sergey Kovalev[1], Eduardo J. H. Lee[3], Nilesh Awari[1], Bert Green[1], Susanne C. Kehr[2], Michael Gensch[1], and Lukas M. Eng[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf. Bautzner Landstraße 400, D-01328 Dresden — [2]Technische Universität Dresden. Nöthnitzer Straße 61, D-01187 Dresden — [3]. Universidad Autónoma de Madrid. Calle Francisco Tomás y Valiente 7, E-28049, Madrid

Nanoscopy in the deep THz regime is particularly interesting as the interactions leading to THz resonances, absorption or emission (i.e. interactions of spins, lattice, and charge carriers) are occurring on a much smaller length scale as compared to the wavelengths of the corresponding electro-magnetic fields. As the tool of choice, scattering-type scanning near field optical microscopy (s-SNOM) at THz wavelengths was previously demonstrated with superb spatial resolution when operated in the time domain. In this talk we report on the implementation of s-SNOM for time-domain-spectroscopy and nanoimaging near or even under the Nyquist-Shannon sampling limit, using broadband table-top sources and a unique accelerator-based super-radiant THz light source at low-repetition-rate (1 - 200 kHz). Operation at low repetition rates is of great importance for a variety of pump-probe experiments, which require THz probing at few 100 kHz or lower, since the typical recovery time after optical excitation in many interesting material systems can be on the order of a few μs.

O 40: Semiconductor substrates: Adsorption

Time: Tuesday 15:15–15:45 Location: MA 005

O 40.1 Tue 15:15 MA 005

Defect density dependence of partial oxidation and deoxygenation reactions of small organic compounds on rutile TiO_2 (110) surfaces — •Lars Mohrhusen, Milena Osmić, and Katharina Al-Shamery — Carl von Ossietzky University of Oldenburg, Institute of Chemistry, D-26129 Oldenburg, Germany

Though titanium dioxide is among the most interesting (photo-) catalyst materials, many structural details of the occurring thermic and photo-stimulated reactions remain unclear. For our mechanistic studies under ultra-high vacuum (UHV) conditions we use a rutile TiO_2 (110) single crystal surface to investigate the adsorption and reaction of small organic molecules such as methanol or methylamine with respect to the defect density.

Defect states like bridging oxygen vacancies as well as Ti^{+III} interstitials can easily be introduced to this material via argon ion sputtering and subsequent annealing in UHV. Around 300 K the Ti^{+III} interstitials start to be mobile and can diffuse towards the surface. We shall present our latest results illustrating the importance of such diffusive bulk defects for thermal reactions of organic molecules such as deoxygenation C-C coupling reactions or partial oxidation in different temperature regimes for alcohols in comparison to amines. Furthermore, we demonstrate the importance of different oxygen species present at the surface for these reactions, using low energy electron diffraction (LEED), temperature programmed desorption spectroscopy (TPD) and in addition Fourier-transformation polarized infrared reflection-absorption spectroscopy (FT-IRRAS).

O 40.2 Tue 15:30 MA 005

Predicting the surface phase diagram of redox-active adsorbates on semiconductor surfaces: The case of ZnO — •Matti Hellström and Jörg Behler — Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammanstr. 6, 37077 Göttingen

We propose an efficient method for calculating surface phase diagrams for redox-active adsorbates on semiconductors, that we apply to the important example of proton (H^+) and hydride (H^-) adsorbates on a ZnO surface [1]. We identify the leading cause for the coverage dependence of the adsorption energies to be the filling and depletion of the disperse substrate conduction band. From only four DFT calculations, coupled with an analysis of the substrate electronic band structure and changes in the electrostatic potential within the substrate upon adsorption, we derive a phenomenological model that well describes the coverage-dependent adsorption energies. We expect that such models can be applied to a wide range of semiconductor substrates and redox-active adsorbates.

[1]. M. Hellström, J. Behler. *Phys. Chem. Chem. Phys.* **19** (2017) 28731

O 41: Poster: Metal Substrates - Structure, Epitaxy, Growth and Adsorption

Time: Tuesday 18:15–20:30 Location: Poster A

O 41.1 Tue 18:15 Poster A

Surface Chemical Bond of a Non-Alternant Aromatic Molecule on Metal Substrates — •Lukas Ruppenthal[1], Benedikt P. Klein[1], Nadine J. van der Heijden[2], Markus Franke[3], Claudio K. Krug[1], Stefan R. Kachel[1], Phil Rosenow[1], Francois Posseik[3], Martin Schmid[1], Ralf Tonner[1], Ingmar Swart[2], Christian Kumpf[3], and J. Michael Gottfried[1] — [1]FB Chemie, Philipps-Universität Marburg, Germany — [2]Debye Insitute, Utrecht University, The Netherlands — [3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany

Metal/organic interfaces have a large impact on the performance of organic-electronic devices, which makes their understanding an important target in surface science. Up to now, the focus has been almost exclusively on aromatic systems with alternant topology such as pentacene, which have a uniform charge distribution and highly delocalized frontier orbitals. In contrast, non-alternant aromatic systems have non-uniform charge distributions and more localized frontier orbitals. These properties are potentially interesting for organic electronics. In this contribution, we present a systematic study of the non-alternant aromatic molecule azulene on the (111) surfaces of Cu and Ag and compare it to its alternant counterpart naphthalene on the basis of NEXAFS, UPS, TPD, nc-AFM, STM and NIXSW measurements. Periodic DFT calculations confirm that the non-alternant topology results in much stronger interaction with metal surfaces, especially in the case of Cu(111), and that the resulting surface chemical bond is more localized.

O 41.2 Tue 18:15 Poster A

spontaneous formation of a superconductor-topological insulator $HfTe_3$ - $HfTe_5$ layered heterostructure — •yuqi wang[1,2], xu wu[1,2], ye-liang wang[1,4], shao yan[1], tao lei[3], jia-ou wang[3], shi-yu zhu[1], haiming guo[1], ling-xiao zhao[1], simin nie[1], hong-ming weng[1,4], kurash ibrahim[3], xi dai[1,4], zhong fang[1,4], and hong-jun gao[1,4] — [1]Institute of Physics, Chinese Academy of Sciences, Beijing, P. R. China — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [3]Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, P. R. China — [4]Collaborative Innovation Center of Quantum Matter, Beijing, P. R. China

Recently, 2D materials and their heterostructures have shown unusual properties. In particular, $HfTe_5$ films and bulk $HfTe_3$ are reported to be 2D large-gap topological insulators (TIs) and superconductors (SCs), respectively. Such a heterostructure made of an s-wave SC and a TI is potentially suitable for studying amazing phenomena including Majorana Fermions. Here we report fabricating a SC-TI heterostructure with a layered configuration of $HfTe_3/HfTe_5$ [1]. The structure of the heterostructure has been determined by STM and XPS. STS measurements reveal a band-gap as large as 60 meV in the HfTe5 film and a SC spectrum in $HfTe_3/HfTe_5$ film. Our current method of making desired heterostructures is based on a spontaneous formation process using surface reactions. This method may provide new routes for the development of other functional heterostructures and nanodevices. References 1. Y. Wang et al., Adv. Mater, 28, 5013 (2016).

O 41.3 Tue 18:15 Poster A

IV-LEED investigations of Ag(001): experimental effects and data analysis — •Jascha Bahlmann, Frederic Timmer, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany

IV-LEED is a powerful technique for surface sensitive structure analysis since the electrons of the used energy range provide information of only the few topmost surface layers. For a successful IV-LEED analysis, it is crucial to know the influences of the experimental setup like the angle of incidence of the electron beam or the temperature of the sample as well as the subtleties in data evaluation.

These effects were investigated systematically for the well known

Ag(001) surface. Especially, we examined their influence on IV-curves recorded in the energy range 50-700 eV and studied the effect on the Pendry R-factor and the resulting geometrical structures determined by IV-LEED analysis. Low temperatures and a well known angle of incidence are essential for reliable results. Additionally the Debye-Waller factor and the root mean square of the thermal displacement of atoms were determined. Furthermore the influence of different filters for the smoothing of experimental spectra was evaluated.

O 41.4 Tue 18:15 Poster A

Investigation of Fe/W(110) system with Field Emission Scanning Probe Microscopy — •Robin Pröbsting[1], Gabriele Bertolini[1], Danilo Andrea Zanin[1], Hugo Cabrera[1], Urs Ramsperger[1], Danilo Pescia[1], and Oguzhan Gürlü[1,2] — [1]Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland — [2]Istanbul Technical University, Department of Physics, 34469 Istanbul, Turkey

We studied the structural and electronic properties of atomic layer iron films on clean and carbide covered W(110) crystal surfaces. Surface structures were studied first by scanning tunnelling microscopy (STM). By means of retracting the tip several nanometres from the sample and increasing the tip bias with respect to the sample, we are able to measure field emitted current both on the tip and on the sample side of the junction. Also, secondary electrons (SE) generated on the sample were collected with a channeltron. Secondary electron maps of the surfaces acquired simultaneously with the absorbed current maps revealed that the local electronic nature of the iron-tungsten system is much richer than the STM shows. The nanometre lateral resolution attained in SE maps and the measurement of the image potential states on different surface locations presents the Topografiner as a potential candidate for atomic level spectroscopy on surfaces.

O 41.5 Tue 18:15 Poster A

Surface crystallography of large organic molecules on metal and insulator surfaces by LEED-IV using Fourier coefficients — •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

We will report on LEED-IV analysis of the large organic molecules PTCDA and NTCDA on the metal and insulator surfaces Ag(100), Ag(111), and KCl(100). Using data from different angles of electron incidence and optimizing the LEED-IV program code we were able to extend the experimental data set and shorten the calculation times required for the complex and large unit cells. Furthermore, the distortion of the PTCDA molecule and the buckling of the Ag surface were described by Fourier coefficients taking into account the symmetry of the system [1]. The idea of this procedure is to suppress unphysical vertical displacements of atoms on a short-wave-length scale by restriction to lower order coefficients.

By this, we obtain good Pendry R-factors, for PTCDA/Ag100 of about 0.23. We were able to derive the vertical distortions of the oxygen atoms in the functional group and the buckling of the Ag surface in rather good agreement with earlier results from DFT and NIXSW studies.

[1] W. Moritz et al, Phys. Rev. Lett. 104, 136102 (2010).

O 41.6 Tue 18:15 Poster A

One-dimensional molecular chain of Co(TAP) on Au(111) — •Cen Yin — Peking university, beijing, China

combined scanning tunneling microscopy(STM), scanning tunneling spectroscopy (STS),) and tip molecular manipulation technique have employed to systematically explore on-surface properties of Co(TAP), as summarized in the following. On Au (111), the Co(TAP) molecules form two kinds of one-dimensional molecular chains. One is the bent chains that bend at the elbow points of the substrate and gradually disappear with the increase of its coverage. The other is the straight one-dimensional chains which adopt three specific surface orientations forming an obtuse angle of 120o against each other at low coverage. At high coverage, the straight molecular chains will not vanish. Variations of the assmeemblye structures with experimental conditions.On Au(111), the assembly structure is more seriously affected by temperature than by the coverage . At liquid nitrogen temperature, the Co(TAP) molecules form one-dimensional chains along the herringbone troughs eventually two-dimensional assembly structure at full coverage. On Ag (111), three co-existing assemblies the assembllies formed and are not affected by coverage and temperature. On Cu(111), the two-dimensional assembly structure appears only if the surface covrage reaches nearly full coverage.

O 41.7 Tue 18:15 Poster A

First principles investigations on the electronic structure of mercaptocarboxylic acids adsorbed on ZnO surfaces — •Dennis Franke[1], Michael Lorke[1], Andreia Luisa da Rosa[2], and Thomas Frauenheim[1] — [1]Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Universidade Federal de Minas Gerais, Dept. of Physics, Brazil

Scientific interest in devices consisting of organic and inorganic materials has grown over the past years. Such devices based on nanostructures are very sensitive to adsorbed compounds due to their large surface to volume ratios. In this work we investigate the electronic properties of mercaptocarboxylic acids (MPA) SH-(CH$_2$)$_n$-COOH adsorbed on ZnO-(10$\bar{1}$0) surfaces via density functional theory calculations (DFT) using semi-local and hybrid exchange-correlation functionals. Previous DFT based results have shown that functionalizing the ZnO surface with a thiol group leads to molecular states inside the band gap. We find two possible binding modes for the thiol group on the surface, a monodentate and a bridge mode. We study the influence of both binding modes for different lengths of the methylene chain (n=1, 2, 4, 5, 7) on the density of states (DOS) and the dielectric function to draw conclusions about the possibility to tune the optical properties of ZnO nanostructures.

O 42: Poster: Organic-Inorganic Hybrid Systems and Organic Films

Time: Tuesday 18:15–20:30 Location: Poster A

O 42.1 Tue 18:15 Poster A

Intermolecular Repulsion at Metal/Organic Interfaces: A Quantitative TPD Study — •Stefan Renato Kachel, Benedikt P. Klein, Maik Schöniger, Mark Hutter, Martin Schmid, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Understanding the interaction of π-conjugated organic molecules with metal surfaces is crucial for the development of modern organic electronic devices. Recently we showed how the topology of the π-system influences the surface chemical bond using the example of the structural isomers azulene and naphthalene on Ag(111) and Cu(111) investigated by TPD and DFT calculations. On Cu(111), azulene has a much higher desorption temperature (520 K) than naphthalene (340 K) in the limit of low coverage, while the difference is smaller on Ag(111). With increasing submonolayer coverage, all systems show substantial peak broadening towards lower temperatures. This effect is most pronounced for azulene on Cu(111), where the monolayer signals spread over almost 300 K, adn reveals strong intermolecular repulsion. Two different approaches towards obtaining information about the desorption energy spreading over a monolayer and the strength of the repulsion are presented. Both the Persson model and the inverted Polanyi-Wigner equation are in good agreement with constant-coverage methods like heating-rate variations in the low-coverage range. These studies provide zero-coverage desorption energies of 170 kJ/mol for azulene and 100 kJ/mol for naphthalene, both on Cu(111). Nearest-neighbor repulsion energies for the four systems will be reported.

O 42.2 Tue 18:15 Poster A

Benzene on Ag(111) and Cu(111): A quantitative TPD study — •Janika Hochstrasser, Lukas Hellweg, Stefan Renato Kachel, Martin Schmid, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

The quantitative understanding of metal-organic interfaces is an important prerequisite for the further rational improvement of organic electronic devices, in which these interfaces occur at the electrode/semiconductor contacts. One of the most important single parameter for the quantitative characterization of the metal-organic interaction is the adsorption energy, which can be determined by precision temperature-programmed desorption (TPD) experiments via the desorption activation energy. Such energies represent valuable benchmark data for comparison with computational studies. Here, we focus on benzene as an aromatic model compound and study its interaction with Ag(111) and Cu(111) surfaces. Using an advanced TPD setup with a cryoshroud housing around the mass spectrometer enables us to detect exclusively molecules with a direct line-of-sight path between sample and ion source. The highly precise desorption energies obtained with this setup will be compared with previous experimental and theoretical results.

O 42.3 Tue 18:15 Poster A

Modification of aromatic self-assembled monolayers by electron irradiation: basic processes, related applications, and electric transport properties — Can Yildirim[1], Eric Sauter[1], Andreas Terfort[2], and •Michael Zharnikov[1] — [1]Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [2]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, 60438 Frankfurt, Germany

The effect of electron irradiation on aromatic thiolate self-assembled monolayers (SAMs) with oligophenyl, acene, and oligo(phenylene ethylene) backbones was studied, with emphasis on the basic irradiation-induced processes, performance of these films as negative resists in electron lithography, and electric transport properties. All films exhibited similar behavior upon the irradiation, with clear dominance of cross-linking. The cross-sections for the modification of the SAM matrix, the damage of the SAM-substrate interface, and irradiation-induced cross-linking were derived. Limitations for lithographic applications of these films were considered. The electric transport properties of the SAMs were found to be affected strongly by electric irradiation, with their resistance increasing progressively, by 2-3 orders of magnitude, upon irradiation with doses up to 40 mC/cm2. This increase stemmed predominantly from a change of the contact resistance which, in its turn, was predominantly attributed to progressive irradiation-promoted adsorption of airborne molecules at the SAM-ambient interface. Based on the transition voltage spectroscopy, the behavior of the HOMO-LUMO gap upon irradiation was monitored.

O 42.4 Tue 18:15 Poster A

Investigation of Metal-Organic Interfaces by Adsorption Calorimetry — •Maik Schöniger, Martin Schmid, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg

Measuring heats of adsorption and reaction by desorption-based techniques such as temperature-programmed desorption (TPD/TDS) is more challenging than it might seem at first view, because even small organic molecules such as benzene decompose before they desorb from reactive surfaces such as Pt(111). In these cases, where irreversible adsorption occurs, TPD fails. Instead, direct calorimetric measurements of the heats released during adsorption have to be performed. The same is true for adsorption processes which have an activation barrier. With our adsorption calorimeter, heats of adsorption and reaction can be determined directly for a large variety of systems, including the adsorption of metals and organics on metal surfaces or the reaction of metals with organic films. Metal-organic interface energies are of special importance for the design and development of future organic electronic devices such as organic light-emitting diodes (OLEDs) or organic solar cells (OSCs). Here, we discuss interfaces of low work function electrode metals such as Ca with organic semiconductors. Besides the interface energies, we also obtained data on the transmittance of thin metal films for IR radiation.

O 42.5 Tue 18:15 Poster A

Metal-Phthalocyanines on Noble Metal Surfaces: A Systematic Investigation With Respect to Strong Correlation Effects — •Manuel Grimm, Dennis Hein, Christian Metzger, Martin Graus, Achim Schöll, and Friedrich Reinert — Exp. Physik 7, Universität Würzburg, 97074 Würzburg, Germany

Metal-organic interfaces provide an ideal playground to study fundamental interaction mechanisms. In particular cases, these can lead to electronic correlations which cannot be described within a single particle picture. In case of some adsorbate/substrate combinations the LUMO of molecules in the first layer is partially occupied due to charge transfer from the metal substrate. As a result such samples, e.g. NTCDA or CuPc on Ag(111) [1,2] show a sharp Kondo resonance at the Fermi energy in high resolution photoelectron spectroscopy (PES) experiments. Here we present a systematic study of these resonance features. We analyze the influence of sample temperature and vary the bonding strength and charge transfer at the interface by changing the adsorbate and the orientation of the substrate surface. While we observe a Kondo scenario for NiPc and CuPc on Ag(111) which is explained within a Single Impurity Anderson model (SIAM), a more complicated behavior occurs on Ag(100) and Ag(110) surfaces. In the latter cases the NiPc and CuPc LUMO is still partially filled at room temperature, but starts to shift to larger binding energies upon cooling. This also leads to a shift of the sharp resonance peak away from the Fermi energy, which demands for an explanation beyond the SIAM.

[1] Schoell *Science* 329, 303 (2010) [2] Ziroff *PRB* B85 (2012)

O 42.6 Tue 18:15 Poster A

Photoisomerization characteristics of azobenzene-functionalized SAMs/Au(111) — •Wibke Bronsch, Larissa Boie, Thomas Moldt, Jan Böhnke, Beatrice Andres, Daniel Przyrembel, Cornelius Gahl, and Martin Weinelt — Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin

Self-assembled monolayers (SAMs) of azobenzene-functionalized alkanethiolates form molecular ensembles with preferential orientation and significant excitonic coupling among the azobenzene chromophores. It has been under debate if the excitonic coupling influences the *trans*-*cis* photoisomerization of the azobenzene units in the ensemble. In this contribution we use the sensitivity of the sample work function on the density of *trans* and *cis* isomers [1] to investigate this question by means of two-photon-photoemission. The photon-energy dependence of the photostationary state and the effective isomerization cross-sections in SAMs with different azobenzene content allows for disentangling different excitation pathways. It turns out that predominantly localized excitations contribute to photoswitching while the contribution of intermolecular coupled and thus delocalized excitonic states is minor [2].

[1] W. Bronsch, D. Przyrembel, L. Boie, C. Gahl and Martin Weinelt, *Fast optical work-function tuning at an organic/metal interface*, Appl. Phys. Lett. **111**, 081601 (2017)

[2] W. Bronsch, T. Moldt, L. Boie, C. Gahl and Martin Weinelt, *Delocalized versus localized excitations in the photoisomerization of azobenzene-functionalized alkanethiolate SAMs*, J. Phys.: Condens. Matter **29**, 484002 (2017)

O 42.7 Tue 18:15 Poster A

STM investigation of organic molecules on a Dy-Ag surface alloy — •Sina Mousavion, Johannes Seidel, Lu Lyu, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

One of the great goals in the field of molecular adsorbates is to control the electronic and geometric structure at metal-organic interfaces. While most studies so far focused on modifications of the organic film to tune the interfacial properties, we have started to tailor metal-organic interfaces by surface alloying [1].

Here, we extend this approach to new surface alloy consisting of silver and lanthanide metal, Dysprosium grown on a silver crystal . The lateral order of the bare Dy1Ag2 surface alloy is characterized by LEED and STM and reveals a reveals a Sqrt(3)xSqrt(3) structure with an additional Moiré pattern. Subsequently, the structure formation and lateral order of PTCDA and the single molecular magnet Sc3N@C80 are investigated. We find a clear correlation between the local arrangement of the molecular adsorbates and the Moiré pattern of the surface alloy.

[1] Phys. Rev. Lett. 117 096805 (2016)

O 42.8 Tue 18:15 Poster A

Towards Computational Structure Prediction of Organic Thin Films and Multilayers: TCNE on Cu(111) — •Alexander T. Egger, Lukas Hörmann, Andreas Jeindl, Michael Scherbela, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Austria

Organic thin films often crystallize in peculiar, surface-induced phases, which exhibit physical properties that are superior to the bulk structures. However, resolving the surface-induced thin film phases remains a huge challenge, in particular for first-principle calculations. While efficient structure determination strategies exist for isolated molecules or bulk crystals - and to a limited extend also molecular monolayers

- none of these are efficiently applicable to multilayer structures or organic thin films.

In this contribution, we demonstrate a strategy to fill this gap. Using the SAMPLE approach, which combines coarse-graining of the potential energy surface with machine learning, we start from an energetically optimized first layer. Subsequently, we predict energetically favorable positions for a single molecule in the second layer. Using these positions as "building blocks", we create a new discretized PES to predict structure of higher layers.

Here, we demonstrate the applicability of this approach on TCNE (tetracyanoethene) on Cu(111). Specifically, we investigate whether, at high coverage, the system will undergo a phase transition from a densely packed, face-on geometry to upright standing molecules, or whether - and in which structure - a TCNE bilayer forms.

O 42.9 Tue 18:15 Poster A

Molecular dynamics simulation of transport and nucleation of conjugated organic molecules on inorganic surfaces — Mila Miletic, Joachim Dzubiella, and •Karol Palczynski — Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany

In our study we analyze the influence of polarity on the surface transport and nucleation of conjugated organic molecules on the inorganic amorphous SiO_2 and ZnO surfaces by means of all-atom molecular dynamics simulations. In particular, we thoroughly investigate the effects of partial fluorination of the popular para-sexiphenyl (*p*-6P) molecule with chemical modifications of one head group (*p*-6PF2) or both head and tail (*p*-6PF4). Even though the chemical modifications do not lead to significant changes in the molecular structure, the effect of the fluorination on the diffusion process on the ZnO substrate is considerable, leading to a difference in the diffusion barriers of one order of magnitude between *p*-6P and *p*-6PF4. However, in case of the amorphous SiO_2 substrate, the difference in the diffusion barriers between *p*-6P and *p*-6PF2 is negligible. To fully understand the effects that controll the diffusion mechanisms, our aim is to investigate the relation between the surface barriers and the underlying surface dynamics, as well as to characterize substantial contributions of entropy to the effective diffusion barriers. Furthermore, we employ molecular dynamics simulations to identify the sources of nanometer-scale disorder in organic crystal structures on inorganic substrates.

O 42.10 Tue 18:15 Poster A

Interfaces of solution processable doped organic transport layers with metals and conductive oxides — •Patrick Reiser[1,2], Eric Mankel[1,2], and Wolfram Jaegermann[1,2] — [1]Institute for Materials Science, Technische Universität Darmstadt — [2]InnovationLab GmbH Heidelberg

Employing printing and solution processing of organic films has the potential to reduce manufacturing costs and to enable large scale flexible organic devices. A key to maintain high performance is given by proper interface engineering of printed layer towards the electrode material. Buffer layers or doped organic transport layers are used to create Ohmic contacts, which generally improves device performance. Here, we investigated the energetic and electrochemical properties of a doped hole transport material like P3HT and Spiro-OMeTAD towards electrodes like ITO or Silver by means of Photoelectron Spectroscopy. We further compare vacuum and solution processed films as well as the deposition sequence.

O 42.11 Tue 18:15 Poster A

Towards accurate prediction of ground state charge transfer with Fermi-Löwdin orbital self-interaction corrected DFT — •Torsten Hahn[1], Simon Liebing[1], Martin Knupfer[2], Mark Pederson[3], and Jens Kortus[1] — [1]TU Freiberg, Institute for Theoretical Physics, Germany — [2]IFW Dresden, Electronic and Optical Properties Department, Germany — [3]Johns Hopkins University, Department of Chemistry, USA

Organic charge transfer (CT) compounds are a class of materials that allow tuning of electronic and optical properties by controlling the amount of charge that is transferred between a donor and acceptor molecule. Accurate predictions of properties of CT materials based on calculations within the density functional theory (DFT) framework are challenging and often result in unsystematic fails.

The application of the recently proposed Fermi-Löwdin orbital self-interaction correction [1,2,3] scheme (FLO-SIC DFT) to CT compounds containing TCNQ and related acceptor molecules leads to significant improvements of the theoretical results compared to experimental data.

[1] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[2] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)
[3] T. Hahn et. al., J. Chem. Phys., vol- 143, 224104 (2015)

O 42.12 Tue 18:15 Poster A

Orbital Imaging of Non-Planar Molecules Beyond the Free Electron Finalstate Approximation — •Christian Metzger, Manuel Grimm, Martin Graus, Achim Schöll, and Friedrich Reinert — Julius-Maximilians-Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg, Germany

It has been shown that the imaging of molecular orbitals is possible by angle-resolved photoelectron spectroscopy (ARPES). For planar aromatic molecules the approximation of the photoemission final state by a simple plane wave allows for a particularly straightforward interpretation of the experimental data. Here we present a combined experimental and theoretical study on the angular intensity distribution of photoelectrons from non-planar molecules. The ARPES data of a single layer of C60 on Ag(110) was acquired by a momentum microscope which enables the efficient detection of photoelectrons emitted into the entire hemisphere above the sample. The symmetry of the recorded photoelectron momentum maps (PMM) immediately demonstrates that the molecules adsorb with a single specific alignment and do not rotate even at room temperature. On the theoretical side, a simple plane-wave approximation of the finalstate is bound to fail due to the 3D geometry of C60. A more suitable description can be realized within the framework of independent atomic centers (IAC), where the finalstate can be assembled by the composite contributions of the individual atoms inside the molecule. We demonstrate that this IAC approach provides a very good simulation of the experimental PMM and thus allows the assignment of different initialstate orbitals.

O 42.13 Tue 18:15 Poster A

Interactions in Hybrid Nanocomposite Systems studied by Laser-Induced Photoemission Electron Microscopy — •Kevin Oldenburg[1], Christian Völkner[1], Johannes A. A. W. Elemans[2], Karl-Heinz Meiwes-Broer[1], Sylvia Speller[1], and Ingo Barke[1] — [1]University of Rostock, Institute of Physics, 18059 Rostock, Germany — [2]Radboud University Nijmegen, Institute for Molecules & Materials, NL-6525 AJ Nijmegen, The Netherlands

Utilizing the plasmonic properties of metal nanoparticles to locally create excitons in organic semiconductors is a promising pathway to transfer energy from a defined starting point over long distances. By means of spatially and energetically resolved Photoemission Electron Microscopy (PEEM) we study two nanocomposite systems consisting of mass-selected silver nanoparticles (≈15 nm diameter) on top of Cu porphyrin [1] and of tetracene aggregates, respectively. In case of Cu porphyrin we observe an enhancement of the photoemission signal in the direct vicinity of the nanoparticles. Contributions of electrons from particles versus dye can be clearly distinguished, based on spectral information. In tetracene an additional long lived state is populated which shows both enhanced and decreased population nearby different nanoparticles. The results are discussed in view of particle-molecule aggregate coupling (see also [2]). Open questions concern the dynamics and possible exciton migration as well as annihilation.

[1] H. Hartmann et al., J. Phys. Chem. C 120, 16977 (2016)
[2] K. Stallberg et al., J. Phys. Chem. C 121, 13833 (2017)

O 42.14 Tue 18:15 Poster A

Steering the growth of multiple ordered heteromolecular phases by utilizing intermolecular repulsion — Caroline Henneke, Janina Felter, F. Stefan Tautz, and •Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany and Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

Metal-organic interfaces and their structural, electronic, spintronic and thermodynamic properties have been investigated intensively, aiming to improve and develop future electronic devices. In this context, heteromolecular phases add new design opportunities simply by combining different molecules. However, controlling the desired phases in such complex systems is a challenging task. Here, we report an effective way of steering the growth of a bimolecular system composed of adsorbate species with opposite intermolecular interactions, repulsive and attractive, respectively. The repulsive species forms a two-dimensional lattice gas, the density of which controls which crystalline phases are stable. Critical gas phase densities determine the constant-area phase diagram that describes our experimental observations, including eutectic regions with three coexisting phases. We anticipate the general validity of this type of phase diagram for binary systems containing twodimensional gas phases, and also show that the density of the gas phase allows engineering of the interface structure.

O 42.15 Tue 18:15 Poster A

Analysis of normal incidence X-ray standing wave data considering non-dipolar effects — Markus Franke, Gerben van Straaten, Giuseppe Mercurio, François C. Boquet, Serguei Soubatch, F. Stefan Tautz, and •Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany and Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

Normal incidence x-ray standing wave (NIXSW) is the most established technique for determining the vertical structure at interfaces and surfaces with sub-Angstrom accuracy and chemical sensitivity. However, non-dipolar contributions to the photoemitted electron yield are an issue, in particular since normal incidence conditions are in practice never met. An angle-dependent data analysis is indispensable. In the absence of user-friendly and well-documented software we developed the program "Torricelli" for analyzing NIXSW data. It is open-source, python-based and has an easy-to-use graphical user interface. Data output in an Argand-diagram is included.

O 42.16 Tue 18:15 Poster A

Structural investigation of highly ordered incommensurate monolayer domains of C_{60} on Ag(111) — •Marco Gruenewald, Philipp Müller, Falko Sojka, Jari Domke, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena

We structurally investigated monolayers of C_{60} on Ag(111), which have been prepared by annealing of multilayers, by means of low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). We find that depending on the annealing temperature either the well-known commensurate $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$ structure [E. I. Altman and R. J. Colton, Phys. Rev. B **48**, 18244 (1993)] or previously unknown incommensurate phases are formed. More precisely, a whole family of differently rotated structures could be observed for the latter with domain angles quasi-continuously ranging from 0° to 13.2° while the other unit cell parameters are essentially unaltered compared with the commensurate phase. By means of STM we find that the molecules appear differently rotated on the surface, most likely owing to their inequivalent adsorption sites.

O 42.17 Tue 18:15 Poster A

Thermal stability and interlayer exchange processes of MePc-PTCDA heterostructures on Ag(111) — •Sebastian Thussing and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

The growth and thermal stability of organic heterolayers containing PTCDA and either CuPc or TiOPc have been investigated. Thereby the adsorption geometry and layering of individual species is derived from IR absorption spectroscopy. Information regarding long range order is obtained from SPA-LEED data. Throughout all processing a parallel orientation of the π-conjugated backbone of the deposited molecules is found. Thermal stability of the original layering and the produced organic-organic interface depends crucially on the nature and sequence of deposited species. Heterolayer interfaces involving PTCDA contact layers show excellent stability due to the favorable adsorption energy per unit area for PTCDA in comparison to the phthalocyanines [1]. Another key observation is that all layers comprising double layers of the face-to-face oriented TiOPc species display particular high resistance with respect to thermal annealing, i.e. regarding interlayer exchange and desintegration of the double layer membrane.

[1] S. Thussing and P. Jakob, J. Phys. Chem. C 121 (2017) 13680-13691.

O 42.18 Tue 18:15 Poster A

Morphology and luminescence of tetracene micro- and nanostructures — •Cordelia Horns, Christian Völkner, Mohammadraza Bahrami, Kevin Oldenburg, Regina Lange, Sylvia Speller, and Ingo Barke — University of Rostock, Institute of Physics, 18059 Rostock, Germany

Tetracene is a promising material for long-range exciton transport [1, 2, 3]. We are interested in the transport and coupling of excitons in nanostructured molecule materials. Since fluorescence is one of the possible channels for exciton decay, spatial mapping of fluorescence is a valuable approach for the analysis of excitation pathways. In this work we report on the morphology and luminescence of mesoscopic and nanoscopic tetracene aggregates created by drop-casting on a variety of substrates such as sapphire and glass. We use a correlative approach where the morphology is measured by Atomic Force Microscopy at the same location as fluorescence images within a single microscope, thus avoiding sample transfers. The aggregates exhibit different shapes including morphologies with distinct heights of ~ 30 nm and ~ 100 nm, showing different fluorescence intensity and polarization. By analyzing the images possible reasons and mechanisms for the dependence of fluorescence on the local environment are discussed.

[1] SR Yost, E Hontz, S Yeganeh, T Van Voorhis, J. Phys Chem C, 116, 17369 (2012)

[2] GM Akselrod, PB Deotare, NJ Thompson, J Lee, WA Tisdale, MA Baldo, VM Menon, V Bulovic, Nature Comm. 6, 1 (2014)

[3] X Xie, H Ma, ChemistryOpen, 5, 201 * 205 (2016)

O 42.19 Tue 18:15 Poster A

Multiscale Modeling of ion-sensitive sensor devices — •Jörg Buchwald, Leonardo Medrano Sandonas, Arezoo Dianat, Rafael Gutiérrez, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials Dresden University of Technology, 01069 Dresden, Germany

For the purpose of ion-sensing we want to apply the concept of a reservoir computer. Main part of this device will constitute a network of sensors, that are in contact with the ionic solution (reservoir). To understand the properties of the reservoir computer, knowledge about individual IV characteristics of each sensor is needed. A good candidate for such a sensor is the ion-sensitive field effect transistor (ISFETs). The ISFET can be considered as a FET in which the gate is in contact with an ionic solution and covered by a self-assambled monolayer of biomolecules that are able to bind to specific kinds of ions. The number of bound ions determines the gate potential and the current of the FET. It is assumed to be a function of ion concentration and controlled by binding kinetics.

A good candidate for SAM molecules constitutes the neuropeptide oxytocin, which is able to bind to different types of divalent metal ions. We will employ Molecular Dynamics as well as DFT calculations to scrutinize conformal changes and kinetic stability upon ion binding. From these information we are able to develop a sensor model in which the conformal changes determine the maximum response of the FET gate.

O 42.20 Tue 18:15 Poster A

On the inner structure of porphyrin nanoaggregates revealed by luminescence polarization — •Jannis Becker, Mohammadreza Bahrami, Sven Kraft, Christian Völkner, Kevin Oldenburg, Ingo Barke, and Sylvia Speller — University of Rostock, Institute of Physics, 18059 Rostock, Germany

For studying exciton pathways in molecule nanostructures we prepared copper-based porphyrin aggregates on various surfaces by self-assembly from a solution [1,2]. Apart from the morphology also the inner structure of such aggregates is of interest, particularly for the interpretation of optical and electronic properties in the context of first-principles theory. We address this topic by mapping the luminescence polarization directions of such aggregates. This provides information on the orientation of the transition dipoles and thereby on the orientation of the molecules within the aggregates. We find a pronounced orientation preference for lengthy, tree-like structures, while for more isotropic island morphologies the degree of order is lower. Based on the results we discuss possible structural motifs for the tree-like aggregates.

[1] Hartmann et al., J. Phys. Chem. C 120, 16977 (2016).

[2] Bahrami et al.: Correlative Microscopy of Morphology and Luminescence of Cu porphyrin aggregates, submitted.

O 42.21 Tue 18:15 Poster A

A versatile facility for time-resolved multidimensional spectroscopy of few-layer surface systems in a nanostructured environment — •Sebastian Pres[1], Bernhard Huber[1], Emanuel Wittmann[2], Daniel Fersch[1], Lysanne Dietrich[1], Julian Lüttig[1], Victor Lisinetskii[1], Matthias Hensen[1], Eberhard Riedle[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Lehrstuhl für BioMolekulare Optik, Ludwig-Maximilians-Universität, Oettingenstraße 67, 80538 München, Germany

We present here a surface spectroscopy setup which combines aberration-corrected photoemission electron microscopy (AC-PEEM), enabling sub-5 nm spatial resolution, with a widely tunable highrepetition-rate (up to 1 MHz) laser source. Organic and inorganic few-layer systems can be directly prepared and characterized in-situ by low-energy electrons (LEEM, LEED) and ex-situ by scanning fluorescence microscopy. Tuning of the optical excitation from 900 nm down to 230 nm at sub-25 fs pulse duration allows a precise spectral addressability of sample specific resonances. The laser pulses, used in collinear time-interferometric scanning schemes like two-colour pump-probe techniques, reveal surface dynamics in 2D materials, e.g., WSe2. Further, the usage of amplitude- and phase-shaped pulse sequences permits the investigation of transport processes between and within individual molecules in organic-inorganic hybrid systems by space- and time-resolved multidimensional spectroscopy.

O 42.22 Tue 18:15 Poster A

III/V-on-Si(100) heterointerfaces and single-domain virtual substrates — •Oliver Supplie[1], Benjamin Borkenhagen[2], Oleksandr Romanyuk[3], Toma Susi[4], Matthias M. May[5], Sebastian Brückner[1], Agnieszka Paszuk[1], Andreas Nägelein[1], Peter Kleinschmidt[1], Michael Rienäcker[2], Gerhard Lilienkamp[2], Winfried Daum[2], and Thomas Hannappel[1] — [1]Institute of Physics, TU Ilmenau, Germany — [2]Institute of Energy Research and Physical Technologies, TU Clausthal, Germany — [3]Institute of Physics, ASCR Prague, Czech Republic — [4]Faculty of Physics, University of Vienna, Austria — [5]Chemistry Department, Cambridge University, UK

Pseudomorphic virtual GaP/Si substrates are attractive for III/V-on-Si integration. Adequate preparation of the GaP/Si(100) heterointerface is of particular interest since its atomic and electronic structure highly impacts crystal quality. Here, we present experimental results regarding the formation of the GaP/Si(100) heterointerface from optical in situ studies during metalorganic vapor phase epitaxy and in system photoelectron spectroscopy. These are discussed with respect to recent results from density functional theory [PRB 94:155309 (2016); PRL 118:237403 (2017)]. Specific changes in the MOVPE process routes enable modifications of the atomic structure at the heterointerface. In particular, we study the influence of As and Ga. We correlate these experiments to reference experiments, where Si surfaces are exposed to Ga and P in UHV and the impact on the surface structure is studied in situ with low energy electron microscopy (LEEM).

O 43: Poster: Semiconductor Substrates - Adsorption

Time: Tuesday 18:15–20:30 Location: Poster A

O 43.1 Tue 18:15 Poster A

Preparation and characterization of monolayer Thallium films on Si(110) — •Pascal Grenz[1], Philipp Eickholt[1], Anke Beck-Schmidt[1], Koji Miyamoto[2], Kazuyuki Sakamoto[3], and Markus Donath[1] — [1]Westfälische-Wilhelms-Universität Münster, Germany — [2]Hiroshima Synchroton Radiation Centre, Japan — [3]Department of Nanomaterials Science, Japan

Surface states of thin Thallium-layers on Sillicon are strongly influenced by spin-orbit-interaction (SOI), leading to peculiar spin textures. One example is the Tl/Si(110)-(1x1) surface with C_1h symmetry a non vortical Rashba spin structure in the occupied states has been observed[1]. For the unoccupied states a large spin splitting along $\bar{\Gamma}\bar{X}$ with an out-of-plane spin polarization is predicted. A well prepared surface is cruical for the investigation of the unoccupied electronic structure with spin- and angle-resolved inverse photoemission (SRIPE). In this contribution, we present different preparation methods and discuss the influence of those on the crystallographic and electronic surface structure.

[1] E. Annese *et al.*, Phys. Rev. Lett. **117**, 016803 (2016)

O 43.2 Tue 18:15 Poster A

Preparation and Characterization of a Monolayer Thallium on Si(110) — •Pascal Grenz[1], Philipp Eickholt[1], Anke Beck-Schmidt[1], Koji Miyamoto[2], Kazuyuki Sakamoto[3], and Markus Donath[1] — [1]Instiute of Physics, Westfälische-Wilhelms-Universität Münster, Germany — [2]Hiroshima Synchroton Radiation Centre, Japan — [3]Department of Nanomaterials Science, Chiba University, Japan

Surface states of thin thallium-layers on silicon are strongly influenced by spin-orbit-interaction (SOI) leading to peculiar spin textures. One example is the Tl/Si(110)-(1x1) surface, with C_{1h} symmetry, where a non vortical Rashba spin structure in the occupied electronic states has been observed [1]. For the unoccupied states a large spin splitting along $\bar{\Gamma}\bar{\mathrm{X}}$ with an out-of-plane spin polarization is predicted.

A well prepared surface is cruical for the investigation of the unoccupied electronic structure with spin- and angle-resolved inverse photoemission (SRIPE). In this contribution, we present different preparation methods and discuss the influence of those on the crystallographic and electronic surface structure.

[1] E. Annese *et al.*, Phys. Rev. Lett. **117**, 016803 (2016)

O 43.3 Tue 18:15 Poster A

Preparation and Characterization of a Monolayer Thallium on Si(110) — •Pascal Grenz[1], Philipp Eickholt[1], Anke Beck-Schmidt[1], Koji Miyamoto[2], Kazuyuki Sakamoto[3], and Markus Donath[1] — [1]Instiute of Physics, Westfälische-Wilhelms-Universität Münster, Germany — [2]Hiroshima Synchroton Radiation Centre, Japan — [3]Department of Nanomaterials Science, Chiba University, Japan

Surface states of thin thallium layers on Si(111) are strongly influenced by spin-orbit-interaction leading to peculiar spin textures [1]. A further interesting example is the Tl/Si(110)-(1x1) surface, where a nonvortical Rashba spin structure was observed in the occupied electronic states at **k**-points with C_{1h} symmetry [2]. For the unoccupied states, a large spin splitting is predicted along $\bar{\Gamma}\bar{\mathrm{X}}$ with an out-of-plane spin polarization. A well-prepared surface is crucial for the investigation of the surface bands. In this contribution, we report on different preparation methods and discuss their influence on the crystallographic and electronic surface structure.

[1] S.D. Stolwijk *et al.*, Phys. Rev. Materials **1**, 064604 (2017)

[2] E. Annese *et al.*, Phys. Rev. Lett. **117**, 016803 (2016)

O 43.4 Tue 18:15 Poster A

Hexacene generated by deoxygenation on passivated silicon — •Frank Eisenhut[1], Justus Krüger[1], Dmitry Skidin[1], Seddigheh Nikipar[1], José M. Alonso[2], Enrique Guitián[2], Dolores Pérez[2], Dmitry A. Ryndyk[1,3], Diego Peña[2], 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]Centro de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS) and Departamento de Química Orgánica, Universidade de Santiago de Compostela, 15782-Santiago de Compostela, Spain — [3]Bremen Center for Computational Materials Science (BCCMS), Universität Bremen, 28359 Bremen, Germany

On-surface synthesis represents a successful strategy to form designed molecular structures on an ultra-clean metal substrate. On non-metallic substrates, on the other hand, on-surface synthesis would allow the electrical decoupling of the resulting molecule from the surface, making possible the application of this powerful synthesis approach to electronics and spintronics. Here, we demonstrate that the on-surface generation of hexacene by surface-assisted reduction, already observed on Au(111), can be performed on the H-passivated Si(001) surface. The reaction, observed by scanning tunneling microscopy, is probably driven by the formation of Si-O complexes on the dangling bond defects. Supported by DFT calculations, we investigate the interaction of hexacene with the passivated silicon surface, and with single silicon dangling bonds.

O 43.5 Tue 18:15 Poster A

Cobalt-Pyrphyrin on $\mathrm{Cu_2O(111)}$: A promising system for photocatalytic water splitting — •Lisa Grad, Fabio Cossalter, Wolf-D. Zabka, Stephan Schnidrig, Benjamin Probst, Roger Alberto, Zbynek Novotny, Matthias Hengsberger, and Jürg Osterwalder — University of Zurich, Winterthurerstrasse 190, 8057

Zurich, Switzerland

Photocatalytic water splitting presents a sustainable way to store solar energy in the form of chemical bonds. For large-scale use, the combination of molecular catalysts supported on abundant substrates is a viable approach. We investigate one such model system: Cobalt-Pyrphyrin (CoPyr) [1] adsorbed on the Cu$_2$O(111) surface.

Cu$_2$O(111) is a p-type semiconductor with downward band bending. This property is conserved after adsorbing a layer of CoPyr [2]. The related electrical field supports charge separation by accelerating excited electrons from the Cu$_2$O to the interface from where they can relax to unoccupied states of CoPyr. There are two different reconstructions of the Cu$_2$O(111) surface observed: (1x1) and ($\sqrt{3}\times\sqrt{3}$)R30°. The structure and stoichiometry of these different surface reconstructions and their influence on electrical properties are still not fully understood, but are expected to influence the surface band bending and charge carrier dynamics. Our current effort centers on investigation of these properties using angle-resolved X-ray photoelectron spectroscopy and time-resolved two-photon photoemission.

[1] Joliat et al., Dalton Transactions 2016 45(4), 1737-1745

[2] Leuenberger et al., Nano Letters 2017 17 (11), 6620-6625

O 43.6 Tue 18:15 Poster A

The adsorption and dimererisation of Co-Salen molecules on NaCl(100) — •Rasmus Jakobsen — University College London, London, United Kingdom

In this work, we investigate the interactions of magnetic molecules with bulk insulating surfaces. These systems are of interest due to their potential uses in fields such as molecular electronics and magnetism. In particular the self-assembly of the transition metal-organic complex of Co-Salen ((Co(C16H14N2O2)) with the NaCl(100) surface, is investigated. Experimentally, this have been measured using non-contact atomic force microscopy (NCAFM) by our collaborators A. Schwarz at University of Hamburg. Co-Salen is deposited and adsorbed as individual molecules onto NaCl(100). However, room temperature measurements show two different morphologies consisting of Co-Salen dimer building blocks; a nanowire and nanocrystallite structure. How these structures form and the reasons for their relative stabilities is unknown. In previous studies, Density Functional Theory (DFT) was used to provide an unambiguous determination of the adsorption geometry of a single molecule. To continue this work, the self-assembly process has been investigated using a combined approach of DFT, semi empirical methods and empirical force fields, studying various aspects of the system such as the adsorption process of multiple molecules, step adhesion and dimerization of the molecule on the surface.

O 44: Poster: Oxide and Insulator surfaces: Structure, Epitaxy, Growth and Adsorption

Time: Tuesday 18:15–20:30 Location: Poster A

O 44.1 Tue 18:15 Poster A

Formation of cobalt ferrite on SrTiO$_3$(001) by Interdiffusion of Fe$_3$O$_4$/CoO bilayers — •Jannis Thien, Jari Rodewald, Martin Hoppe, Karsten Küpper, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

Ultrathin epitaxial cobalt ferrite (CoFe$_2$O$_4$) films are in the focus of both spintronics and spin caloritronics since they combine semiconducting properties with ferrimagnetic properties and high Curie temperature. Therefore, cobalt ferrite films can be used as spin filters [1] or as supports for Pt films which are used to obtain deeper insight into the Spin Seebeck effect (SSE) [2].

One approach to prepare ultrathin CoFe$_2$O$_4$ films is reactive solid phase epitaxy where the interdiffusion of Fe$_3$O$_4$/CoO bilayers is used. Therefore, Fe$_3$O$_4$/CoO bilayers were consecutively grown by reactive molecular beam epitaxy on SrTiO$_3$(001). Afterwards, the samples were post-annealed at different temperatures. The effects of interdiffusion were examined after each annealing step by means of x-ray reflectivity (XRR), soft x-ray photoelectron spectroscopy (Soft XPS), hard x-ray photoelectron spectroscopy (HAXPES) and x-ray diffraction (XRD) using synchrotron radiation.

XRR, Soft-XPS as well as HAXPES revealed interdiffusion of Fe$_3$O$_4$ and CoO layers after an annealing temperature of 673K and probable formation of Co$_x$Fe$_{3-x}$O$_4$ layers with $0.4 \leq x \leq 1$.

[1] J.-B. Moussy, J. Phys. D: Appl. Phys. 46, 143001 (2013)

[2] K. Uchida et al., Nature (London) 455, 778-781 (2008)

O 44.2 Tue 18:15 Poster A

Temperature dependent spin polarization in EuO thin films investigated by high resolution ARPES — •Tristan Heider[1,2], Timm Gerber[1], Patrick Lömker[1], Claus Michael Schneider[1,2], Lukasz Plucinski[1,2], and Martina Müller[1,3] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [3]Experimentelle Physik I, TU Dortmund, 44227 Dortmund, Germany

The ferromagnetic insulator EuO is predicted to show 100% spin polarization at the valence band maximum, which makes this material a prototype candidate for research in the field of spintronics. Our goal is to interface it with a topological insulator to introduce time-reversal symmetry breaking without an external magnetic field.

As a first approach we studied MBE growth of EuO on Cu(001), because Cu is a very good electrical conductor, thus, ideally suited as an aid for charging problems in band mapping from an insulating thin film. After we could narrow down the EuO synthesis to a very small parameter window, in which single-crystalline growth is mastered, we performed temperature dependent high resolution spin-ARPES measurements. A non-vanishing spin polarization of the O 2p band as well as up to 52% in the Eu 4f band could be obtained. Furthermore the temperature dependence of the Eu 4f polarization can be described by the Brillouin function and confirm the literature value of $T_C = 69$ K.

O 44.3 Tue 18:15 Poster A

Ni on Fe$_3$O$_4$: Post deposition annealing treatments and Ni diffusion into Fe$_3$O$_4$ — •Andreas Alexander, Martin Hoppe, Joachim Wollschläger, and Karsten Küpper — Fachbereich Physik, Universität, Barbarastr. 7, 49076 Osnabrück, Germany

One approach of preparing the magnetic insulating ferrite NiFe$_2$O$_4$ is the interdiffusion of Fe$_3$O$_4$/NiO bilayers [1]. Very recently, it has been demonstrated that the surface properties of spinel ferrites can be precisely controlled by diffusion of metallic Co into Fe$_3$O$_4$ [2]. Here we study the diffusion of metallic Ni into Fe$_3$O$_4$. We have grown Ni/Fe$_3$O$_4$ by reactive molecular beam epitaxy (RMBE) on SrTiO$_3$(001). Then the samples were post-deposition annealed (PDA) at three different temperatures, i.e. 400°C, 500°C, and 700°C, in UHV and 10^{-4} mbar O$_2$ to tackle the diffusion process. The structural surface characterization was performed by low energy electron diffraction (LEED) after each PDA step, whereas x-ray photoelectron spectroscopy (XPS) was employed to investigate the surface chemical composition. In order to gain information about the Ni incorporation into the bulk of the magnetite layer, we employed hard x-ray photoelectron spectroscopy (HAXPES) due to its enhanced electron escape depth. HAXPES was performed at the beamline I09 of DLS.

[1] O. Kuschel et al., Phys. Rev. B 94, 094423 (2016).

[2] R. Gargallo-Caballero et al., J. Chem. Phys. 144, 094704 (2016.)

O 44.4 Tue 18:15 Poster A

Corundum surface energies from DFT and MD simulations — •Lilit Amirkhanyan, Hemanth Nagaraj, and Jens Kortus — TU Freiberg, Institute for Theoretical Physics, Germany

The surface energy is a very important property for a broader understanding of materials features. The knowledge of oxide surfaces like e.g. Al$_2$O$_3$ is essential to understand crystal growth, corrosion or sintering phenomena.

We examined the surface energy of the stable α - Al$_2$O$_3$ using first principles density functional theory (DFT) and molecular dynamics (MD) simulation.

This is a study of α - Al$_2$O$_3$ relaxed surfaces, surface energies. Our results indicate possible growth planes and interfaces which may have implication for morphology or catalytic behaviour.

O 44.5 Tue 18:15 Poster A

The Growth and Fluorescence of Phthalocyanine Monolayers and Thin Films on Hexagonal Boron Nitride — •Manal

Alkhamisi, Vladimir Korolkov, and Peter Beton — School of Physics & Astronomy, University of Nottingham, Nottingham NG7 2RD, U.K.

We have investigated the adsorption of metal-free phthalocyanine (Pc) thin films on hexagonal boron nitride (hBN) using high resolution atomic force microscopy under ambient conditions. The Pc molecules are sublimed onto hBN under vacuum conditions. A set of samples were grown at room temperature with wide range of film thickness (0.2nm-32nm) and the effect of temperature variation of the substrate was also investigated. At low coverage, metal-free phthalocyanine form needle-like islands in which the molecules are coplanar with the substrate. With increasing thickness in the range 4nm to 32nm the morphology of the islands changed to form dendritic-like disordered islands which are attributed to cofacial stacking of molecules. At growth temperatures close ~100 oC we observe the formation of large monolayer islands and we are able to obtain AFM images with molecular resolution from which we can identify the packing and ordering of the molecules. The photoluminescence of the Pc films was measured with a fluorescence microscope and we find a very intense red-shifted zero-phonon peak for the monolayers with additional peaks for multilayer samples which appear at lower energy and are close to those observed for Pc powder. We discuss these red shifts in relation to substrate and intermolecular interactions.

O 44.6 Tue 18:15 Poster A

Surface terminations of oxidized Nb(110), from Nb$_2$O$_5$ to NbO$_{1\approx x}$ — •Kuanysh Zhussupbekov[1], Brian Walls[1], Killian Walshe[1], Emma Norton[1], Sergey I. Bozhko[2], Karsten Fleischer[1], Andrey M. Ionov[2], Valery N. Semenov[2], and Igor V. Shvets[1] — [1]School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College, University of Dublin, Dublin 2, Ireland — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia

The oxidation of single crystalline Nb(110) is investigated by low-energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM) and spectroscopy (STS). Oxidizing at low temperature and/or high oxygen partial pressure results in the formation of Nb$_2$O$_5$. STM measurements reveal an amorphous surface which is found to be insulating by STS measurements. Annealing in ultra-high vacuum (UHV) above 700^oC removes this native oxide and sees the formation of NbO$_{x\approx1}$ surface [1]. This surface is characterized by stick-shaped NbO$_{x\approx1}$ nanocrystals. The terrace step width is defined by the nanocrystal stick length and one-dimensional terrace states are observed by STS measurements. Ion bombardment of this surface and subsequent annealing forms a NbO$_{x\approx1}$ surface with a different terrace structure. Finally, the oxidation of the NbO$_{x\approx1}$ nanocrystal surface is investigated; room temperature oxidization and subsequent UHV annealing results the extra oxygen sitting in between the NbO$_{x\approx1}$ nanocrystals.

[1]. I. Arfaoui et al., Physical Review B 65, 115413 (2002).

O 44.7 Tue 18:15 Poster A

Acetone on the TiO$_2$ rutile surfaces: Adsorption, reaction and IR spectra — Tim Würger[1], Wolfgang Heckel[1], •Kai Sellschopp[1], Heshmat Noei[2], Yuemin Wang[3], Andreas Stierle[2,4], Stefan Müller[1], and Gregor Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]DESY NanoLab, Deutsches Elektronensynchrotron, Hamburg — [3]Institute of Functional Interfaces, Karlsruhe Institute of Technology — [4]Physics Department, Hamburg University

Acetone is often present in chemical reactions during the formation of hybrid interfaces, and thus is a potential competitor to coupling agents like carboxylic acids. Moreover, acetone can be oxidized via photo-catalysis at TiO$_2$ surfaces. Here, we studied the adsorption geometry, energetics and vibrational modes of acetone molecules on the TiO$_2$ rutile (110) surface with density functional theory (DFT) and IR spectroscopy. Studying a large number of possible adsorption geometries in DFT calculations, we found that even at high coverage the adsorbed acetone is able to change its configuration by thermal activation. IR spectra were recorded while dosing acetone on rutile powder particles at low temperature and agree very well with the calculated IR spectra. Increasing the temperature resulted in a reaction of the adsorbed acetone. The nature of this reaction is examined using DFT.

O 44.8 Tue 18:15 Poster A

LEED I(V) analysis of the physisorption system C$_2$H$_2$ $(3\sqrt{2}\times\sqrt{2})$R45°/NaCl(100) — •Jochen Vogt — Chemisches Institut der Uni Magdeburg, Magdeburg, Germany

The first layer acetylene adsorbed on the NaCl(100) surface is known to form long-range ordered structures with $(3\sqrt{2}\times\sqrt{2})$R45° and $(7\sqrt{2}\times\sqrt{2})$R45° translational symmetry, respectively [1,2]. The comparatively large unit cells in this system are assumed to be induced by a moderate lattice mismatch with the substrate. In both cases, however, the adsorbate structure is not known in full detail. The poster presents first results of an I(V) structure analysis for the $(3\sqrt{2}\times\sqrt{2})$R45° phase. Calculated full dynamical LEED intensities are fitted to experimental data of seven diffraction spot orders. An unusual feature of the in-house search algorithm for R-factor minima is the use of rigid molecule structure parameters instead of individual atomic site coordinates, with the advantage of a reduced number of free parameters. According to LEED (Pendry R-factor=0.27), the substrate exhibits a small site specific surface rumpling. The acetylene molecules are placed in average 2.71 Å above the Na$^+$ ions in a nearly parallel orientation with respect to the surface plane. Lattice mismatch induced strain appears to be released by small lateral shifts of the molecules from the exact on-top positions over Na$^+$.

[1] A. Glebov, R. Miller, J. P. Toennies, J. Chem. Phys. **106** (1997) 6499. [2] A. G. Cabello-Cartagena, J. Vogt, H. Weiss, J. Chem. Phys. **132** (2010), 74706.

O 45: Poster: Solid-Liquid Interfaces - Structure, Spectroscopy, Reactions and Electrochemistry

Time: Tuesday 18:15–20:30 Location: Poster A

O 45.1 Tue 18:15 Poster A

Observation of material movement on KBr surfaces depending on the relative humidity — •Dominik Kirpal, Korbinan Pürckhauer, Alfred J. Waymouth, and Franz J. Giessibl — University of Regensburg, Regensburg, Germany

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

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

O 45.2 Tue 18:15 Poster A

Characterization and Chemical Imaging of Aerosols from remote Antarctica — •Johannes Weis[1,2,6], Ricardo H. M. Godoi[1,3], Ana F. L. Godoi[1,3], Simon Mueller[1,2], Sérgio J. Gonçalves Jr.[3], Heitor Evangelista[4], Swarup China[5], Bingbing Wang[5], Alexander Laskin[5], Tristan H. Harder[6], and Mary K. Gilles[1] — [1]Chemical Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — [2]Department of Chemistry, University of California, Berkeley, CA 94720, USA — [3]Department of Environmental Engineering, Federal University of Paran UFPR, Curitiba, PR, Brazil — [4]LARAMG, State University of Rio de Janeiro Uerj, Rio de Janeiro, RJ, Brazil — [5]William R. Wiley Environmental and Molecular Science Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99352, USA —

[6]Department of Physics, University of Würzburg, Germany

Changes in Antarctica's ice sheets and shelves are of primary concern to the regional and global climate. We hypothesize that the West Antarctic warming can be related to the aerosols transported and formed in this region. Internal composition and characteristics of single aerosol particles were investigated by means of chemical mapping via synchrotron-based scanning transmission X-ray microscopy with near edge X-ray absorption fine structure spectroscopy (STXM/NEXAFS), followed by a rule-based cluster classification. Complementary data obtained from computer-controlled scanning electron microscopy (CC-SEM/EDX) allows us to go a step forward in the understanding of aerosol particles formed in Antarctica's pristine environment.

O 45.3 Tue 18:15 Poster A

A compact and calibratable von Hamos X-Ray Spectrometer based on two full-cylinder HAPG mosaic crystals for high-resolution XES — •Ina Holfelder, Rolf Fliegauf, Yves Kayser, Matthias Müller, Malte Wansleben, Jan Weser, and Burkhard Beckhoff — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany

For high-resolution X-ray Emission Spectroscopy (XES), crystal-based Wavelength-Dispersive Spectrometers (WDS) can be applied for effective speciation characterization of nano- and microscaled materials. A von Hamos geometry provides the highest detection efficiencies combined with high resolving power. This geometry uses a cylindrically bent crystal as dispersive and as a sagittal focusing optic. Highly Annealed Pyrolytic Graphite (HAPG) can be deposited reliably on cylindrical glass substrates and shows highly integrated reflectivity while offering low mosaicity, ensuring high resolving power. A novel calibratable von Hamos X-ray spectrometer based on two full-cylinder optics is being put into operation at the PTB. The spectrometer enables chemical speciation of elements in an energy range from above 10 keV down to 2.3 keV. The first results using synchrotron radiation as the excitation source will be presented. The spectrometer combines high efficiency with high spectral resolution in a compact arrangement also suitable for laboratory arrangements.

O 45.4 Tue 18:15 Poster A

charge accumulation on copper electrode surfaces were studied by means of electrochemical and optical techniques — •Saúl Vázquez-Miranda[1,2], Reza Sharif[1], Kurt Hingerl[1], and Christoph Cobet[1] — [1]Johannes Kepler Universität, Zentrum für Oberflächen und Nanoanalytik, Altenberger Str. 69, 4040 Linz, Austria — [2]Universidad Autónoma de San Luis Potosí ,(IICO) Av, Karakorum 1470, 78216 San Luis Potosí, México

The surface chemistry occurring during electrocatalysis is the key to understand the reaction mechanism.Electrochemical and optical methods were used to investigate the charge accumulation at amorphous and single crystals of Cu surfaces interacting with a supra pure HCl solution.

The investigation of the adsorption/desorption of Cl- ions was carried out using cyclic voltammetry, in which the integrated charge and ion - exchange is measured in a potential window where we prevent damage of the copper surface.

Electrochemical impedance spectroscopy (EIS) measurement on the (111) and (110) faces of copper was used to extract capacitance and resistance parameters. Equivalent circuit modeling was used to suggest the potential of zero charges (PZC).

Spectroscopy Ellipsometry for in operando characterization allows to probe the solid/liquid interface directly while applying an external potential and during chronoamperometry. The correlation of these two techniques allows to shed light on the charge accumulation on the copper surface electrodes.

O 45.5 Tue 18:15 Poster A

The Influence of Li-Imide Salt Additives in Li-Ion Battery Electrolytes on the Solid Electrolyte Interphase Formation on Graphite Electrodes — •Thomas Diemant[1], Varvara Sharova[2,3], Arianna Moretti[2,3], Alberto Varzi[2,3], R. Jürgen Behm[1,2], and Stefano Passerini[2,3] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, Albert-Einstein-Allee 47, D-89069 Ulm — [2]Helmholtz Institute Ulm (HIU) Electrochemic Energy Storage, Helmholtzstr. 11, D-89077 Ulm — [3]Karlsruhe Institute of Technology (KIT), P.O. Box 3640, D-76021 Karlsruhe

The solid electrolyte interphase (SEI), a passivating layer which is formed by electrolyte decomposition during the first electrochemical cycles on the electrodes of Li-ion batteries (LIBs), is one of the main factors influencing the battery performance. In order to ensure the formation of a SEI with well-balanced physico-chemical characteristics, additives are often included into the electrolyte formulation. These additives either decompose prior to the electrolyte main components during the first charge or incorporate into the passive layer, leading to the formation of a more compact, stable and ion conducting SEI.

Herein, we report results of a detailed study on the effect of various Li imide salts (LiTFSI, LiFTFSI, and LiFSI) as electrolyte additives in LIBs, in which the chemical composition and thickness of the SEI layer on graphite anodes is characterized by ex-situ XPS. This is complemented by characterization of the SEI resistance via electrochemical impedance spectroscopy (EIS). Finally, the implications for the cycling performance in half and full cells are discussed.

O 45.6 Tue 18:15 Poster A

Dissolution of noble metals (Au, Ag, Cu) in a trihalide ionic liquid in oxidation state +1 as shown by XPS — •Benjamin May[1], Matthias Lexow[1], Hans-Peter Steinrück[1], Florian Maier[1], Nicola Taccardi[2], Juergen Schatz[3], and Harald Maid[4] — [1]Physikalische Chemie II, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]Chemische Reaktionstechnik, FAU Erlangen-Nürnberg, Erlangen, Germany — [3]Organische Chemie I, FAU Erlangen-Nürnberg, Erlangen, Germany — [4]Organische Chemie II, FAU Erlangen-Nürnberg, Erlangen, Germany

The corrosion of metals, particularly those generally considered inert, is important to many of the applications of trihalides. In this poster we present the results of X-ray photoelectron spectroscopy analysis of a trihalide ionic liquid, $[C_6C_1Im][Br_2I]$, and its reactions with the group 11 metals copper, silver, and gold. We find that all three of the metals are susceptible to corrosion by the IL. In addition, we find evidence that all three metals are dissolved in the +1 oxidation state. We propose a reaction of the general form:

$M + [Br_2I]^- \longrightarrow M^+ + 2Br^- + I^\bullet$,

with two iodine radicals recombining to form molecular iodine. Additional testing shows that this reaction occurs in both the presence and absence of water, and that the imidazolium C2 proton is not involved in the corrosion reaction.

O 45.7 Tue 18:15 Poster A

Chemical analysis of solid-liquid interfaces by in-situ Rutherford Backscattering Spectrometry — •Nasrin B. khojasteh and René Heller — HZDR, Dresden, Germany

Solid-liquid interfaces are important locations for various reactions to occur in biological, chemical and physical processes [1-3]. Recently, an experimental setup for in-situ Rutherford Backscattering Spectrometry (RBS) technique has been installed at the 2 MV Van-de-Graaff accelerator at Ion Beam Center (IBC) of the Helmholtz-Zentrum Dresden-Rossendorf to analyze solid-liquid interfaces as well as to conduct electro-chemistry experiments. The focus of the project is to perform experiments in different fields utilizing this quantitative, non-destructive and standard free ion beam analysis technique for solid-liquid interfaces. A Si3N4 window separates the liquid in the cell from vacuum in the beam line. He+ beam with E = 1.7 MeV is employed to bombard the samples. For feasibility tests, the cell was filled with air, Ne, He, Xe and DIH2O respectively and RBS and Particle Induced X-Ray Emission Spectroscopy (PIXE) spectra were recorded. To examine the efficiency of the technique, ion backscattering studies of the solid-liquid using 0.1M solutions of Cu(NO3) and AgNO3 have been performed and are compared to the literature [4].

[1] Kötz et al., Electrochimica acta. 31 (1986) 169. [2] Morita et al., Radiation Physics and Chemistry. 49 (1997) 603. [3] Hodnik et al., Accounts of chemical research. 49 (2016) 2015. [4] Forster et al., Nuclear Instruments and Methods in Physics Research Section B. 28 (1987) 385.

O 45.8 Tue 18:15 Poster A

Morphology and electronic structure of MnO_2 nanoparticles from first-principles — •Yonghyuk Lee, Jakob Timmermann, Daniel Opalka, and Karsten Reuter — Technische Universität München, Germany

Manganese oxides are characterized by an outstanding variety of stoichiometries and morphologies. Many structures show high catalytic activity in photo- and electrochemical applications. With Mn as one of the most abundant elements this offers great potential for energy related applications. In the present work we consider MnO_2 which has been identified as an efficient anode material in the electrolysis of water. For a first characterization of polycrystalline MnO_2 we employ ab initio thermodynamics to determine the relative stabilities of hydrated and pristine surfaces as a function of the applied potential. Stable MnO_2 nanoparticle structures are predicted on the basis of the Gibbs-Wulff theorem and the electronic band structure of the particles is analyzed as a function of their size and shape dependence.

O 45.9 Tue 18:15 Poster A

Electrolysis of CO_2 at Platinum/Ionic Liquid Interfaces — •Andre Kemna and Björn Braunschweig — Institute of Physical Chemistry, WWU Münster, 48149 Münster, Germany

Electrochemical CO_2 reduction reactions (CO2RR) at Pt(poly) and Pt(111)/electrolyte interfaces were studied with cyclic voltammetry (CV). Using different room temperature ionic liquids (RTIL) as electrolytes such as [BMIM][BF_4] and [EMIM][BF_4], we have investigated the influence of both water and the chemical identity of the RTIL as a co-catalyst on the activity for CO2RR. H_2O concentrations between 0.1 and 2 M lead to a substantial rise in activity. In addition, also the surface structure has a significant impact: Compared to polycrystalline Pt, well-ordered Pt(111) electrodes have a substantially lower activity for CO2RR. In order to study the molecular structure of Pt(poly)/[EMIM][BF_4] interfaces in situ and in more detail, we have applied vibrational sum-frequency generation (SFG)[1]. Potentiodynamic SFG spectra reveal a vibrational mode centered at 2355 cm^{-1} which we attribute to a [CO_2-EMIM] complex at the interface that lifts the inversion symmetry of CO_2 molecules and makes them SFG active. We propose that these interfacial complexes can function as a stable precursor for CO_2 reduction reactions and lead to small overpotentials for CO2RR. Another vibrational band at 2080 cm^{-1} is due to atop CO as the main reduction product of CO_2 electrolysis on Pt surfaces. Strongly adsorbed CO molecules cause a poisoning of the Pt catalyst and lead to a deactivation over many cycles.

[1] B. Braunschweig et. al. J. Electroanal. Chem., 2017, 800, 144-150

O 45.10 Tue 18:15 Poster A

Towards understanding the mechanism of water splitting on TiO2 — Saman Hosseinpour, Simon J. Schlegel, Mischa Bonn, and •Ellen H.G. Backus — Max Planck Institute for Polymer Research, 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 TiO2 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 TiO2. Sum frequency generation spectroscopy (SFG), is an inherently surface sensitive tool, allowing the study of the water-TiO2 interface. As a first step in understanding the water-splitting reaction, we studied the binding of water to the substrate. From the intensity and frequency of the SFG signal we extract information about the binding of water to the TiO2. Moreover, we show time-resolved SFG data after excitation of the TiO2 with a femtosecond UV pump pulse which mimics the sun light. Preliminary data show that both the surface and the interfacial water molecules undergo changes on ultrafast timescales upon excitation. These UV-pump SFG-probe data illustrate the first steps towards following the photo-induced dissociation of water at the TiO2 interface in real-time.

O 45.11 Tue 18:15 Poster A

DFT study of halogen adsorbate structures on the (100) surfaces of Ag and Au in an electrochemical environment — •Alexandra Dávila, Lukas Deuchler, Svenja Hövelmann, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, CAU Kiel, Germany

The electrochemical interface between halide containing electrolytes and coinage metal electrodes constitutes an important model system. The chemical potential of the halogen as a function of sample potential, which is crucial for the theoretical description of various processes at the electrode, is in general derived from thermodynamics. Analogously to previous work for halogens/Cu [1] we present a systematic density functional study [2,3] for Cl, Br, and I adsorption on Ag and Au(100). Our DFT calculations include incommensurate adsorbate reconstructions via large unit cells. Differences between the range of stability of equilibrium reconstruction as a function of sample potential as derived from the calculations and the conditions under which the respective structures have been observed experimentally [4] are identified. Furthermore, the atomic structure of the boundary between c(2×2)-Cl adsorption domains on the unreconstructed Au(100) surface have been calculated and are compared to STM images from [5].

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[3] P. Giannozzi et al., J. Phys. Condens. Matter 21, 395502 (2009).

[4] X. Gao *et al.*, J. Phys. Chem. **98** (1994).

[5] Y.- C. Yang *et al.*, Electrochim. Acta **112** (2013).

O 45.12 Tue 18:15 Poster A

Deposition and reactivity of single Pd clusters at solid-liquid interfaces — •Clara Rettenmaier, Nicolas Bock, Astrid De Clercq, Ueli Heiz, and Friedrich Esch — Chemistry Department & Catalysis Research Center, Technische Universität München, Garching, 85747, Germany

Electrochemical deposition of Pd monolayers on Au(111) have been studied extensively [1]. Palladium shows high catalytic activities for many chemical reactions and is capable to absorb hydrogen. In particular, submonolayer coverages show significant electrocatalytic enhancement for the hydrogen evolution reaction (HER) [2]. However, size-selected Pd clusters in the non-scalable size regime have barely been studied in aqueous environments, despite their potential for high catalytic activities.

We present the preparation of single size Pd clusters on Au(111) by decomposition of polyoxometalates [3] under controlled electrochemical potential and pH. The clusters are characterized by Electrochemical Scanning Tunneling Microscopy (ECSTM) and Rotating Disc Electrode (RDE) measurements, while the HER activity of single clusters is measured in situ using the STM tip as a microelectrode.

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[2] Pandelov, S., Stimming, U., Electrochimica Acta 2007, 52(18), 5548-5555.

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O 45.13 Tue 18:15 Poster A

In situ Video-STM Studies of Sulfide Adsorbate Dynamics on Ag(100) in Iodide Solution — •Reihaneh Amirbeigiarab, Bjoern Rahn, and Olaf M. Magnussen — Kiel University

Atomic scale dynamic processes at the interface between electrodes and electrolyte solutions play a pivotal role in electrochemical phase formation reactions. Accordingly, the evaluation of the atomic scale surface dynamic processes on metal electrodes, such as adsorbate diffusion and interaction, is of great importance to understand the reaction mechanisms at solid/liquid interfaces. In situ video-STM allows direct atomic-scale studies of these highly dynamic processes on electrode surfaces. [1-3] We here present results of in situ Video-STM studies on the dynamic behavior of low coverages of sulfide adsorbates on Ag(100) electrode surfaces in iodide-containing solution. We observe clear differences in the potential-dependend diffusion behavior on surfaces covered by a c(2×2)-I coadsorbate layer and by a disordered iodide adlayer, respectively. Futhermore, restructuring of the Ag substrate is found, leading to nanoscale grooves. The results are compared to previous data for sulfide on c(2×2)-Cl and c(2×2)-Br covered Ag(100). [1] T. Tansel, O. M. Magnussen, Phys. Rev. Lett., 96, 026101. (2006) [2] A.Taranovskyy, T. Tansel, O.M. Magnussen, Phys. Rev. Lett., 104, 106101.(2010) [3] Y. C. Yang, A. Taranovskyy, O. M. Magnussen, Angew. Chem. Int. Ed., 51, 1966. (2012)

O 45.14 Tue 18:15 Poster A

Electrochemical Roughening of Pt(111) : Surface Site Reactivity — •Leon Jacobse[1], Yi-Fan Huang[1], Marcel J. Rost[2], and Marc T.M. Koper[1] — [1]Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands — [2]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands

Most devices that form the basis of an energy sustainable future, rely on platinum electrocatalysts. To optimize the use of this scarce and expensive metal, it is of the utmost importance to understand the catalyst's degradation on the atomic-scale.

We followed the roughening of Pt(111) upon repeated oxidation and reduction cycles (ORCs), by combining simultaneous cyclic voltammetry and in-situ EC-STM. This approach, together with the long timescale of our experiments, reveals new insights on the roughening process. Within the performed 170 ORCs we observe a continuous increase of the electrode roughness that can be separated into two different growth regimes, each of which exhibits their own correlation with the electrochemically measured number of hydrogen adsorption sites. Comparing the average atomic-scale island structure during the evolution with the disentangled voltammetric signals provides insight into the reactivity of the individual surface sites, like steps, kinks, and corner atoms.

[1] L. Jacobse, Y.-F. Huang, M.T.M. Koper, M.J. Rost, Nature Materials, accepted (2017)

O 45.15 Tue 18:15 Poster A

Chemical Functionalization of Oxide Surfaces: Insights into the Mechanism of Molecular Adsorption at the Solid/Liquid Interface — •Paul Schwarz and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Oxide surfaces are usually functionalized by attaching strongly interacting linker groups, like phosphonic acid or silanol units, employing wet-chemical processes. To obtain a fundamental understanding of the binding and reaction mechanisms at the solid/liquid interface we performed ab initio molecular dynamics (AIMD) simulations to study the anchoring of methylsilanetriol (MST) to aluminum oxide surfaces via condensation reactions in the presence of residual water and liquid isopropanol. Applying Thermodynamic Integration (TI) and Umbrella Sampling (US), we calculated the activation barrier for the surface binding of MST. Depending on whether residual water is present or not, the condensation reaction is found to be spontaneous or activated. Spontaneous condensation can proceed in two different ways, either by an initial protonation of an OH group of the surface or of the MST molecule. In the first case, an intermediate six-membered ring between MST and the desorbing water molecule is formed. In contrast, the protonation of an OH group of MST results in a pentacoordinated Si atom, where the surface OH group at the adsorption site is substituting the leaving OH group of MST.

O 45.16 Tue 18:15 Poster A

Electro-oxidation of CO on Au modified planar and nanostructured Pt(111) electrodes — •Evelyn Artmann, Julian Bösking, Jens Klein, Valeria Chesnyak, Albert K. Engstfeld, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm

The catalytic activity of Platinum (Pt) for the oxidation of CO was shown to increase with increasing amount of low coordinated Pt sites, like Pt step edges, on the surface which may be more active compared to terrace sites.[1] The exact role of step sites in the reaction mechanism is, however, still under debate. A strategy to identify the role of Pt steps in the CO oxidation is to block the steps by decorating them with a narrow Au film and then to compare the activity of the electrode with and without Au decoration. Prior to this it is, however, important to investigate the stability of such Au films on Pt as well as the influence of the Au film on Pt terrace sites for the CO oxidation activity. To this end, we first prepared and structurally characterized, by STM under UHV conditions, Pt(111) single crystals with varying Pt step densities. Subsequently, we decorated the Pt steps with monolayer high Au films and varied the Au coverage from sub-monolayer to full monolayer coverage. Investigating the structural characteristics of the surfaces before and after CO oxidation, as measured in an electrochemical flow cell, provided us information about the electrode stability under reaction conditions and about the influence of the Au film at Pt step and terrace sites on the activity of the electrodes for CO oxidation. [1] G. García et al., *ChemPhysChem.* **12** (2011) 2064.

O 45.17 Tue 18:15 Poster A

Deactivation of Hazardous Chemicals at Oxide Surfaces — •Tobias Klöffel[1], Mariana Kozlowska[2], Bernd Meyer[1], and Pawel Rodziewicz[2] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Institute of Chemistry, University of Bialystok, Poland

After World War II, large quantities of highly toxic chemical warfare agents were disposed in the Baltic Sea, where highly corroded containers, nowadays frequently found in fishing nets or at beaches, constitute a major environmental hazard. A very promising approach for the decomposition of the chemical warfare agents is via hydrolysis reactions using oxide catalysts, in particular, ZnO nanorods. Since it is close to impossible to perform standard surface science experiments for such highly toxic materials, *in silico* research is the only alternative for obtaining insights into the chemical processes at the solid/liquid interface leading to defunctionalization. Here, we will present first results on the adsorption and decomposition of sulfur mustard on ZnO surfaces based on Car-Parrinello Molecular Dynamics (CPMD) simulations. The different types of molecule–surface interactions have been analyzed and the mechanism of the first hydrolysis step has been studied using metadynamics for overcoming reaction barriers. All simulations were done for a full water/ZnO interface, which was created by embedding ZnO in several layers of water.

O 45.18 Tue 18:15 Poster A

Electrochemical Surface Science of Magnetite Fe_3O_4 under Oxygen Evolution Conditions — •Matthias Müllner, Michele Riva, Giada Franceschi, Gareth Parkinson, Ulrike Diebold, and Stijn F.L. Mertens — TU Wien, Institut für Angewandte Physik, Wiedner Hauptstrasse 8-10/134, 1040 Vienna

Earth-abundant oxides such as magnetite Fe_3O_4, with the addition of dopants, are promising candidates for an effective but low-cost catalyst for the oxygen evolution reaction (OER), which is one of the remaining bottlenecks in electrolysis and artificial photosynthesis.

We report electrochemical surface science studies on well-defined magnetite single-crystal surfaces, with the aim of linking reactivity to atomic-level structural information. Preparation and characterisation in UHV (STM, LEED, XPS) are followed by transfer to the electrochemical environment (open-circuit potential measurements, cyclic voltammetry, impedance), using a new sessile-drop cell design. Post-measurement characterisation of the surface in UHV and by ambient AFM indicates stability of $Fe_3O_4(001)$ towards electrolyte exposure (pH 7 up to 14) and during OER. Ongoing work aims to reveal the effects of surface orientation, whether transition-metal-doping of the surface is feasible and how this affects electrocatalytic activity.

O 45.19 Tue 18:15 Poster A

A Novel Electrochemistry Flow Cell for Operando Soft X-Ray Spectroscopy on Catalysts: Demonstrated on a MnOx Film for the Water Oxidation Half Reaction — •Marc F. Tesch[1], Shannon A. Bonke[1], Maryam N. Shaker[1], Travis E. Jones[2], Jie Xiao[1], Rosalie K. Hocking[3], and Alexandr N. Simonov[4] — [1]Helmholtz Zentrum Berlin, Berlin, Germany — [2]Fritz-Haber-Institut, Berlin, Germany — [3]Swinburne University of Technology, Victoria, Australia — [4]Monash University, Victoria, Australia

We present a novel flow cell design for soft X-ray spectroscopy on catalysts optimized for in situ electrodeposition and electrochemistry. Soft X-ray based photon-in - photon-out techniques can probe the electronic structure of a catalyst while it is in contact with an electrolyte and a potential is applied, i.e. operando. Soft X-ray absorption spectroscopy (XAS) allows probing the unoccupied valence states, thereby providing information such as the oxidation state of the catalyst. Resonant inelastic soft X-ray scattering (RIXS) can access valence electronic processes such as charge transfer and dd-transitions. The combination of XAS and RIXS provides a comprehensive picture of electronic changes occurring in a catalyst when tuning the external conditions towards its active state, e.g. by increasing an applied potential across the overpotential. The applicability of the aforementioned experimental techniques is demonstrated on a MnOx catalyst for the water oxidation half reaction measured at different applied potentials. The experimental results are discussed with focus on the potential induced changes in its electronic structure and are compared to theory.

O 45.20 Tue 18:15 Poster A

Wetting properties of CuFeO2 delafossite for photo-catalytic processes — Diego Diaz, Robert Wheatley, Martín Roble, Marcelo Cisternas, Donovan Diaz, •Ulrich G. Volkmann, Alejandro Cabrera, Birger Seifert, and Sascha Wallentowitz — Institute of Physics and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile

Metal oxides and ceramics are used universally as catalytic and photocatalytic materials for a very wide range of chemical reaction processes. For water based reactions, hydroxylization, a process dependent upon the wettability of at the surface, can greatly influence catalytic activity of a metal oxide. In this work we present an investigation of the wetting properties CuFeO2 delafossite oxide synthesized using hydrothermal methods. We show how the "as grown" powder produces a strong hydrophobic effect which is described using the Cassie model for suspended droplets upon a rough surface comprised of two materials. Treatment of the powder via milling, pelletization and sintering reveals a hydrophobic surface which is then described by the Wenzel regime. However, in some cases we observe a rapid absorption of the water which we currently attribute to micro-capillaries present in the pellet sample. The material and its surface is characterized via XRD, AFM, FESEM and EDS methods. Acknowledgements: CONICYT Fellowships (MR, MC) and CONICYT-PIA ACT 1409.

O 45.21 Tue 18:15 Poster A

Assets and drawbacks of electrochemical/-catalytic characterization of electrodes prepared under UHV conditions — •Albert K. Engstfeld, Jens Klein, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Our current understanding of the electrochemical/-catalytic properties of complex three dimensional catalyst materials is strongly based on single crystal studies, supported by theoretical studies. In general, the electrochemical properties are characterized on single crystal electrodes prepared under laboratory conditions. These findings are supported by separate UHV studies, in which the electronic and chemical properties of the surfaces are explored by surface sensitive techniques. In order to bridge the gap between UHV and laboratory studies, numerous attempts are presented in the literature over the last decades, where electrochemical techniques are combined with a UHV set-up.[1] In this work, we will first discuss the relevance of the respective approach to prepare single crystals with distinct structural properties under UHV conditions, which can be elucidated with STM measurements and present examples where a clean environment, such as UHV, is indispensable to obtain the respective electrodes. Furthermore, we will present different types of bimetallic structures which can only be formed under laboratory conditions and other types which can only be obtained under UHV conditions. Finally, we will discuss situations where the combination UHV-electrochemistry approach is highly advantageous to in situ electrocatalytic studies. [1] PCCP, 19 (2017) 4141

O 46: Poster: Molecular Films - Photovoltaics, Electronics and Morphology

Time: Tuesday 18:15–20:30 Location: Poster A

O 46.1 Tue 18:15 Poster A

Control of Polymorphic Phases of an Anilino Squaraine by Organic Molecular Beam Deposition — Tobias Breuer[1], Frank Balzer[2], Matthias Schulz[3], Arne Lützen[3], •Manuela Schiek[4], and Gregor Witte[1] — [1]University of Marburg, D — [2]University of Southern Denmark, Sonderborg, DK — [3]University of Bonn, D — [4]University of Oldenburg, D

Squaraines are small molecular quadrupolar donor-acceptor-donor (D-A-D) chromophores absorbing in the red spectral range considered for application as photovoltaic materials [1, 2]. A prototypical anilino squaraine with branched alkyl side chains (SQIB) crystallizes at least into two polymorphic bulk structures. In spin-casted thin films these two phases emerge with a strongly preferred out-of-plane and rather random in-plane orientation upon thermal post-annealing directed by the annealing temperature [3]. Now we investigate the surface induced growth of thermally vapor deposited SQIB on varying dielectric and conductive substrates and correlate the observed polymorphs to the substrate properties. We approach a complete picture of molecular orientation relative to the substrate geometry for instance by X-ray diffraction and polarized light microscopy. [1] Appl. Phys. Lett. 111 (2017) 183502. [2] Langmuir 32 (2016) 8533. [3] Cryst. Growth Des. (2017) DOI: 10.1021/acs.cgd.7b01131.

O 46.2 Tue 18:15 Poster A

single molecule study of ClAlPc on Au(111) Surface with low temperature scanning tunneling microscopy — •Hao Zhu, Wenhui Zhao, Huanjun Song, and Kai Wu — CCME, Peking University, No.5 Yiheyuan Road Haidian District, Beijing, 100871

Chloroaluminum phthalocyanine(ClAlPc), a non-planar molecule with a Cl atom outside of the phthalocyanine plane, presented constant dipole moment. The adsorption behavior of ClAlPc single molecule deposited on Au(111) surface was studied with the technique of STM, STS and dI/dV mapping. ClAlPc adsorbed on Au (111) with three type of conformation, including Cl atom pointing towards the vacuum (U1 and U2) and Cl atom pointing towards the substrate. Different adsorption orientations were observed between the two types of molecules. Moreover, we measured the orbital states of each type of molecules using STS at the center and dI/dV mapping at various sample bias.

O 46.3 Tue 18:15 Poster A

All-carbon nanocapacitors from graphene and carbon nanomembrane heterostructures — •Xianghui Zhang[1], Emanuel Marschewski[1], Paul Penner[1], Thomas Weimann[2], Peter Hinze[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, University of Bielefeld, 33615 Bielefeld, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Molecular self-assembly allows a precise control of material structure and chemical composition. Here we show the fabrication of all-carbon nanocapacitors composed of multilayer stacks of carbon nanomembranes (CNMs) as dielectrics and graphene as conducting electrodes. CNMs were formed from a series of aromatic self-assembled monolayers of phenylthiol homologues, i.e. biphenylthiol, p-terphenylthiol, and p-quaterphenylthiol. The frequency response of nanocapacitors was measured with an LCR meter and the impedance spectra were analyzed with a simple equivalent circuit, in which the graphene strips were modeled as resistors and the CNM dielectric as a dissipative capacitor. A dielectric strength of up to 4 MV/cm and a capacitance density of up to 0.4 μF/cm^2 were determined for multilayer carbon nanomembranes. The heterostructures possess an interfacial capacitance of 0.5 μF/cm^2. These results show the potential of carbon nanomembranes to be used as dielectric components in next-generation molecular electronics.

O 46.4 Tue 18:15 Poster A

Growth morphologies of dipolar nitrogen based oligoacene derivatives on (0001) sapphire — •Aydan Çiçek[1], Aleksandar Matković[1], Markus Kratzer[1], Zhongrui Chen[2], Olivier Siri[2], Conrad Becker[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben, Franz Josef Strasse 18, 8700 Leoben Austria — [2]Aix Marseille Universitè, CNRS, CINaM UMR 7325, 13288 Marseille, France

Oligoacenes (as pentacene) and their derivatives are promising candidates for applications in organic electronics, due to molecular packing that favours charge transport and thus high field-effect mobilities. This study explores growth morphologies of thin-films and sub-monolayers of dihydro-tetraaza-acenes on the surface of sapphire, a technologically relevant gate dielectric. In particular, dihydro-tetraaza-penatacene (DHTA5) and -heptacene (DHTA7) molecules are considered, both exhibit a similar dipolar momentum. The molecules are deposited using a hot wall epitaxy system. As substrate, vicinal (0001) sapphire is used with an average step distance of 50 nm, and step height of 0.2 nm. The morphology of the grown films is investigated ex-situ by atomic force microscopy. Coverages from sub-monolayers to several layers are analysed, and evolution of needle-like and island-like crystallites is examined as a function of the deposition temperature. Moreover, stability of the crystallites is investigated under prolonged exposure to ambient conditions. Our results show that ambient stability, π-π stacking, and layer-by-layer growth all favor DHTA7 for organic field effect transistor applications.

O 46.5 Tue 18:15 Poster A

Advanced ion optics for Controlled Electro Spray Ion Beam Deposition — •Andreas Walz, Karolina Stoiber, Hartmut Schlichting, and Johannes Barth — Physics Department E20, Technical University of Munich, Germany

The world of nanostructures requires precise control of growth of atomically clean films of particles or molecules on well defined surfaces. Most state of the art techniques to produce such layers like Organic Molecular Beam Epitaxy (OMBE) are limited to small and sublimable particles or molecules. Controlled Ion Beam Depostition (CIBD) gives access to more reactive, fragile and thermolabile species including many biomolecules. One approach is the generation of an ion beam via Electro Spray Ionisation (ESI) at near ambient conditions, its subsequent transfer to Ultra High Vacuum (UHV) and the Soft-Landing on a surface. The challenge using CIBD is to effectively overcome pressure differences of several orders of magnitude while preserving a high ion flux for appropriate preparation times. Here we present some advanced ion optics including a modified high-flux stacked ring ion guide, as well as a square wave driven multipole. To guarantee for a highly purified ion beam with precise control over the deposited species a sophisticated Square-Wave Quadrupole Mass Spectrometer with adjustable frequency and nearly unlimited mass range was established. The construction was assisted by a multitude of simulations done with SIMION.

O 47: Poster: Graphene - Electronic Properties, Structure, Adsorption, Intercalation and Doping (joint session O/TT)

Time: Tuesday 18:15–20:30 Location: Poster A

O 47.1 Tue 18:15 Poster A

The effects of defects and disorder on the electronic structure of graphene — •Piotr Kot[1], Jonathan Parnell[2], Sina Habibian[2], Pavel Ostrovsky[1], and Christian Ast[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]University of British Columbia, Vancouver, Canada

We use a real-space nearest neighbor tight-binding model to study the effect of defects on the band dispersion of graphene. We find that defects in graphene either generally preserve the canonical band structure, or disrupt it by separating the two cones creating an "elongated" Dirac point. This second structure greatly resembles the band dispersion of experimentally measured epitaxial graphene. By using a self-consistent T-matrix approximation we find the reason why defects create two distinctly different band structures, by showing that point defects are either resonant or non-resonant in graphene. Adding all these pieces together, we conclude on the cause of "elongation" in epitaxial graphene and the nature of the electronic structure in the "elongated" region finding that this region can not be considered a gap.

O 47.2 Tue 18:15 Poster A

Spin and charge transport in quasi-freestanding epitaxial graphene grown by CVD — •Jantje Schommartz[1,2], Alexey Kaverzin[2], Christoph Tegenkamp[1], and Bart J. van Wees[2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Deutschland — [2]Physics of Nanodevices, University of Groningen, Netherlands

A promising route for the synthesis of homogeneous large-area graphene, suitable for standard device fabrication techniques, is the epitaxial growth of graphene on SiC. In the present work the growth is achieved by chemical vapor deposition (CVD) by using a hydrocarbon precursor for the carbon deposition on the Si-face of the SiC wafer. We study the quasi-freestanding epitaxial CVD graphene (CVD- QFEG) grown on 6H-SiC(0001) by contacting it with ferromagnetic Cobalt electrodes made by electron-beam lithography technique. By standard lock-in techniques we address the charge and spin transport properties independently by local and non-local measurement geometries. To the best of our knowledge, we detect for the first time spin signatures in transport measurements on CVD-QFEG. This study shows that the CVD-QFEG reveals striking differences in spin and charge transport properties compared to CVD epitaxial graphene. We attribute this to the influence of localized states arising from the buffer layer consistent with the measurements performed on epitaxial graphene grown by sublimation.

O 47.3 Tue 18:15 Poster A

Preparation and characterization of high quality stacks of graphene/h-BN/graphite picked up by a mica substrate — •Michael Weimer[1], Tjorven Johnsen[1], Sayanti Samaddar[1], Peter Nemes-Incze[2], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen, Germany — [2]Centre of Energy Research, Institute of Technical Physics and Materials Science, Nanotechnology Department, 2D NanoFab ERC Research Group, Budapest, 1525, POB 49, Hungary

Graphene on h-BN provides a highly mobile two-dimensional electron system (2DES) which can be characterized by scanning tunneling microscopy (STM). In combination with transport experiments, a comparison of global and local properties of the sample is feasible. Such combination requires an ultra clean graphene surface and at least two electrical contacts. Therefore we present a dry and polymer free preparation technique by using a mica substrate. We exfoliate graphite on mica and subsequently pick up h-BN and graphene from a SiO_2/Si chip one after another. Shadow mask evaporation of gold provides clean contacting. Omitting wet chemical methods and polymers enables ultra clean surfaces with low impurity concentration.

O 47.4 Tue 18:15 Poster A

Effect of the carbon 1s core hole on the polarized x-ray spectra of HOPG - theory and experiment — •Dominik Legut[1], Christine Jansing[2], Hans-Christoph Mertins[2], Andreas Gaupp[2], Peter M. Oppeneer[3], Heiko Timmers[4], and Hud Wahab[4] — [1]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [2]FH Mnster, Stegerwaldstr. 39, D-48565 Steinfurt, Germany — [3]Dept. of Physics and Astronomy, Box 530, S-751 21 Uppsala, Sweden — [4]Univ. of New South Wales Canberra, Australia

Bandstructure calculations using the WIEN2K code have been performed to study the polarized x-ray reflection spectra of highly oriented pyrolytic graphite (HOPG). Varying the amount of the included 1s core hole we find that the DFT calculations provide good agreement with experimentally obtained x-ray spectra [1]. The change of x-ray polarization upon reflection of linearly polarized synchrotron radiation can be become as huge as a birefringent rotation of polarization plane of up to 140°, and the polarization changes from linear to nearly fully circular polarization. The best calculated results are obtained for a partial core hole per excitation. The distinct contributions from the A and B sites of HOPG to the spectra are discussed as well.

Refereces: 1. C. Jansing et al, PRB 94, 045422 (2016).

This work was supported by CSF grant No. 17-27790S and Path to Exascale project No. CZ.02.1.01/0.0/0.0 /16_013/0001791.

O 47.5 Tue 18:15 Poster A

Polycyclic molecules with geometrical frustration via pyrolysis on a metal — •Alexandre Artaud[1], Laurence Magaud[2], Kitti Ratter[3], Bruno Gilles[3], Valérie Guisset[2], Philippe David[2], Jose I. Martinez[4], Jose A. Martin-Gago[4], Claude Chapelier[5], and Johann Coraux[2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts Universität zu Kiel, Germany — [2]CNRS, Institut Néel, Grenoble, France — [3]Grenoble INP, SIMAP, Grenoble, France — [4]Materials Science Factory, Instituto de Ciencia de Materiales de Madrid-CSIC, Madrid, Spain — [5]CEA, INAC, PHELIQS, Grenoble, France

The geometry of molecules is a key to several of their properties. In graphene fragments, electron delocalization from one carbon sublattice to the other is frustrated for molecular shapes breaking the balance of sublattices. Optical, electronic, and magnetic properties emerge in this case, but the synthesis of such molecules remains challenging.

Here, a pyrolysis reaction catalysed by the surface of rhenium is investigated using scanning tunneling microscopy and density functional theory. This reaction known to form graphene is found to also yield graphene fragments consisting of well-defined, zigzag-edged polycyclic molecules, some of which have sublattice imbalance. However, they are found in metastable configurations, which is interpreted as a kinetic rather than thermodynamic control of their formation. Hence, metastable molecules are expectedly ubiquitous in graphene growth, and deleterious to achieve perfect graphene. Pyrolysis is conversely a promising route towards molecules with sought-after properties.

O 47.6 Tue 18:15 Poster A

Scanning Tunneling Microscopy and spectroscopy of Au islands on graphene/Rh(111) — •Anne Holtsch and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Using scanning probe techniques we investigated how graphene (gr) electronically interacts with substrates in the presence of metallic islands on top of the gr layer. In the case of rhodium as a substrate, the band structure is significantly altered with respect to freestanding graphene due to the hybridization of its d orbital with the pz orbital of gr [1]. Using scanning tunneling spectroscopy (STS) the influence of Au Islands on top of the gr was investigated. The islands were deposited by in-situ evaporation. Subsequently their relative orientation with respect to the gr lattice was observed by scanning tunneling microscopy (STM). The STS measurements on and in the vicinity of the islands show locally varying electronic properties of the system. The presence of gold induces the opening of a band gap. At the same time there is an increase in conductivity, compared to the conductivities of gold and gr. Measurements show that the increase in conductivity is restricted to that area of the islands which adjoins to the gr. In this case both gr and gold contribute to a increase of the measured tunnel current.

[1] A. Holtsch, T. Euwens, B. Uder, S. Grandthyll, F. Müller, and U. Hartmann, Surf. Sci. 668 (2018) 107.

O 47.7 Tue 18:15 Poster A

Landau quantization in a graphene monolayer on WSe_2 and $NbSe_2$ — •Felix Förschner[1], Lena Stoppel[1], Fabian Paschke[1], Julia Tesch[1], Yuriy Dedkov[2,1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Deutschland — [2]Department of Physics, Shanghai University, 200444 Shanghai, China

By depositing graphene on transition metal dichalcogenides (TMDs), it is possible to alter the electronic properties of graphene [1]. Here we focus on the fabrication of graphene on WSe_2 and $NbSe_2$, which was successfully performed by an adapted wet chemical transfer process. By means of low-temperature scanning tunneling microscopy we investigate the atomic structure of graphene and observe different Moiré structures indicating a successful transfer of graphene onto the TMD. In an external magnetic field, Landau level sequences are observed giving access to the electronic properties of graphene, i.e. doping level, Fermi velocity etc. Detailed analysis of the obtained tunneling spectra shows that each Landau level is split into subpeaks, where the pronounced splitting strength grows with increasing magnetic field. The magnitude of the observed splitting indicates an enhanced spin-orbit interaction strength in graphene due to the presence of the TMD substrate.

[1] Z. Wang *et al.*, Nature Comm. **6**, 8339 (2015).

O 47.8 Tue 18:15 Poster A

Dislocations in bilayer graphene — •Florian Wullschläger, Konstantin Weber, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Dislocations, i.e. one-dimensional line defects, are the main carriers of plastic deformation in 3D crystalline solids. In a recent TEM study it was shown that dislocations even exist in materials as thin as two graphene layers [1]. Using atomistic simulations based on the registry-dependent potential of Kolmogorov and Crespi [2] we show that the properties of dislocations in quasi-2D crystals differ significantly from their 3D counterparts. The step components of the dislocations give rise to a pronounced buckling of the bilayer in order to release strain energy. All dislocations split into equally-spaced partials due to the absence of a stacking fault energy, a peculiar property of bilayer graphene. Finally, in 2D materials the strain energy induced by a dislocation does not diverge with sample size as in 3D, but remains finite. In addition to this structural characterization of 2D dislocations we will show first results on how dislocations move in bilayer graphene and how they are pinned at lattice defects.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spiecker, Nature **505** (2014) 533.
[2] A. Kolmogorov, V. Crespi, Phys. Rev. B **71** (2005) 235415.

O 47.9 Tue 18:15 Poster A

Microscopic investigations of graphene-nickel interactions — •Philip Schädlich, Florian Speck, Adrian Schütze, and Thomas Seyller — Professur für Technische Physik, TU Chemnitz, Reichenhainer Straße 70, D-09126 Chemnitz

In order to realize possible applications of graphene in electronics, it is important to understand the properties of graphene - metal contact interfaces. In this study we investigate the impact of nickel as possible contact material on the underlying graphene.

Graphene samples are grown by sublimation of Si atoms from a 6H-SiC(0001) substrate in Ar atmosphere at ambient pressure [1]. The local graphene coverage is probed by photoemission electron microscopy as well as low-energy electron microscopy (LEEM) and reflectivity (LEER) spectra. The deposition process of nickel is monitored *in-situ* via LEEM. After deposition, LEER spectra indicate a change of the work function in the covered areas while the characteristic interlayer states [2] stay unchanged. The morphology of the deposited nickel layer is revealed by atomic force microscopy, while the thickness was determined by x-ray photoemission spectroscopy. Angle-resolved photoemission spectroscopy confirms an unchanged electronic band structure with the Dirac point located 0.4 eV below the Fermi energy, which is close to values found for bare monolayer graphene on the 6H-SiC(0001) surface.

[1] K. V. Emtsev et al., Nature Materials 8, 203 (2009).
[2] N. Srivastava et al. Phys. Rev. B 87, 245414 (2013).

O 47.10 Tue 18:15 Poster A

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

To fully understand atom-surface interactions, the availability of an accurate full-dimensional potential energy surface (PES) is crucial. High-dimensional neural network potentials have been shown to provide very accurate PESs for a wide range of systems. Here, we develop a neural network potential for H-atom scattering from a graphene sheet. We fit the potential to density functional theory energies calculated on-the-fly in *ab initio* molecular dynamics simulations. We find that the procedure can reliably describe H at graphene, which makes it possible to effectively simulate the scattering for this system in a large range of incidence conditions.

O 47.11 Tue 18:15 Poster A

Influence of atomic-scale dopants on the transport properties of graphene on SiC — •Anna Sinterhauf[1,2], Philip Willke[1], Georg Traeger[1], Davood Momeni Pakdehi[3], Klaus Pierz[3], Hans Werner Schumacher[3], Hans Hofsäss[4], and Martin Wenderoth[1,2] — [1]IV. Physikalisches Institut, Universität Göttingen, Germany — [2]International Center for Advanced Studies of Energy Conversion (ICASEC), Universität Göttingen, Germany — [3]Physikalisch-Technische Bundesanstalt Braunschweig, Germany — [4]II. Physikalisches Institut, Universität Göttingen, Germany

Tailoring the electronic structure of graphene by substitutional doping often additionally changes its transport properties. In order to study the impact of atomic-scale dopants on electron transport, graphene samples were prepared by polymer-assisted sublimation growth (PASG) [1] and doped with nitrogen atoms by low energy ion beam implantation [2]. Using highly resolved scanning tunneling microscopy and potentiometry, we determined the dopant density as well as the local sheet resistance on the nanometer scale. Moreover, the defect resistance at substrate steps was evaluated. Subsequently, the mobility and the mean free path length were estimated and compared for pristine and nitrogen doped PASG graphene. Furthermore, we were able to quantify the impact of nitrogen dopants on the charge transport, which introduce an additional short-range scattering process along with long-range Coulomb scattering. [1] Kruskopf et al., 2D Materials 3, 041002, 2016 [2] Willke et al., Nano Lett. 15(8), 2015

O 47.12 Tue 18:15 Poster A

Variation of the local transport properties of epitaxial graphene caused by the stacking order of 6H-SiC — •Georg Traeger[1], Anna Sinterhauf[1,2], Davood Momeni Pakdehi[3], Philip Schädlich[5], Florian Speck[5], Johannes Aprojanz[4,5], Thomas Seyller[5], Hans-Werner Schumacher[3], Christoph Tegenkamp[4,5], Klaus Pierz[3], and Martin Wenderoth[1,2] — [1]IV. Physical Institute, University of Göttingen, Göttingen, Germany — [2]Internatonal Center for Advanced Studies of Energy Conversion (ICASEC), University of Göttingen, Göttingen, Germany — [3]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [4]Institute for Solid State Physics, University of Hannover, Hannoner, Germany — [5]Institute of Physics, Chemnitz, Chemnitz, Germany

We present a scanning tunneling potentiometer (STP) study on graphene on silicon carbide (6H-SiC(0001)) grown by polymer assisted sublimation growth (PASG). The high homogeneity of the buffer layer, grown by PASG allows for an investigation of the substrate graphene interaction. [1] Highly resolved STP measurements revealed two distinct sheet resistances, which occur in a characteristic pattern. We identified this pattern with the 6H stacking sequence of the substrate and assigned the graphene terraces to different substrate terminations. Park et al. found that these terminations have different polarization charges [2]. According to this findings, we attribute the termination with the highest polarization charge to the graphene sheet with the highest conductivity.

[1] Pakdehi et al., Submitted [2] Park et al., Phys. Rev. B, 1995

O 47.13 Tue 18:15 Poster A

Ru - mediated growth of graphene on SiC for radiation sensing application — •Rajesh Kumar Chellappan, Simon Cooil, Marina Jorge, Håkon Røst, and Justin Wells — Center for Quantum Spintronics, Norwegian University of Science and Technology, Norway

Graphene has been proposed as a suitable candidate for photo/radiation sensors primarily because of its exceptional electronic properties. However, this advantage has been difficult to realize because of the problems associated with the preparation of high quality graphene on dielectric/semiconductor substrates. Therefore, this study focuses on addressing epitaxial ruthenium mediated graphene growth on silicon carbide and the subsequent interface oxidation using soft X-ray photoemission spectroscopy (SXPS). The growth of graphene and formation of ruthenium silicide was investigated by systematic annealing of ruthenium (˜1nm) deposited on silicon carbide samples in vacuum at temperatures ranging from 450°C to 700°C. The interlayer oxidation was achieved by exposing the sample at 460°C to oxygen partial pressure of 9.5*10-7 mbar for 1 hour to form a graphene/dielectric/silicon carbide device structure.

O 48: Poster: 2D Materials beyond Graphene: TMDCs, Silicene and Relatives

Time: Tuesday 18:15–20:30 Location: Poster A

O 48.1 Tue 18:15 Poster A

Chemical and electronic decoupling of organic molecules by a monolayer of hexagonal boron nitride — •Christine Brülke[1], Timo Heepenstrick[1], Ina Krieger[1], Xiaosheng Yang[2], Simon Weiss[2], Frank Stefan Tautz[2], Serguei Soubatch[2] und Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn — [2]Peter Grünberg Institut, Forschungszentrum Jülich

Hexagonal boron nitride (hBN) is a widely studied material due to its similarity to graphene and its properties as a wide band-gap insulator. We report on the ability of one monolayer hBN to electronically and chemically decouple one monolayer of PTCDA from the Cu(111) surface. Using spot profile analysis low energy electron diffraction (SPA-LEED) and scanning tunneling microscopy (STM) we find a big similarity of the PTCDA monolayer to the (102) plane of the bulk crystal. Investigations via photoelectron spectroscopy (XPS and UPS) show electronic decoupling of the molecules from Cu(111) by the hBN monolayer. The HOMO of the monolayer is located at -2.5 eV below E_F, in accordance with previous findings for multilayers of PTCDA. Normal incidence standing wave experiments (NIXSW) reveal that the vertical binding distance of PTCDA to the hBN layer is very large (3.38 Å) and that the out-of-plane distortion of the molecule is very minute (< 0.1 Å). This points to a weak physisorptive bonding in contrast to the chemisorptive bonding found for PTCDA on Cu(111).

O 48.2 Tue 18:15 Poster A

Epitaxial Growth and Air-stability of Monolayer Antimonene — •xu wu[1,2], yan shao[1], hang liu[1], yeliang wang[1], jiatao sun[1], zhongliu liu[1], shixuan du[1], and hongjun gao[1] — [1]Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

The investigation of two-dimensional (2D) materials has developed rapidly in recent years, inspired by their unique properties and the promise of applications. Recently, many theoretical papers have reported a honeycomb lattice of antimony atoms with expected applications in electric and photoelectric devices [2], called antimonene[1].Here we report the growth of a monolayer of antimonene on layered PdTe2 substrates by epitaxy[3]. Combining our experimental and theoretical results, we verifed that the antimonene is a 2D continuous monolayer with weak coupling to the substrate. Moreover, our fndings reveal that the antimonene is quite inert with respect to air. The monolayer antimonene with its large bandgap and chemical stability is promising for applications in nanoelectronic devices.

[1] S. Zhang et al., Angew. Chem. Int. Ed. 54, 3112 (2015).
[2] G. Pizzi et al., Nat. Commun. 7, 12585 (2016).
[3] X. Wu et al., Adv. Mater. 29, 1605407 (2017).

O 48.3 Tue 18:15 Poster A

Coupling of plasmonic metasurfaces to WS$_2$ monolayers — •Florian Spreyer[1], Feng Shun[2], Yu Ting[2], and Thomas Zentgraf[1] — [1]Universität Paderborn, Paderborn, Germany — [2]Nanyang Technological University, Division of Physics and Applied Physics, Singapore

Recent studies show great potential for transition metal dichalcogenides (TMD) and their optical application. By downscaling TMD's to a single layer flake of atomical thickness, like it is done with graphene, TMD's become semiconductors with a direct band gap. In the past years, new ways of fabrication provided greater flake sizes and higher quality of single layer flakes. Here we study hybrid metasurfaces by combining TMD monolayer flakes with plasmonic nanostructures. We present recent results of the characterization of tungsten disulfide (WS$_2$) flakes transferred to different substrates. By using photoluminescence and AFM measurements we locate monolayers of WS$_2$ and determine their thickness. In addition, metasurfaces made of plasmonic gold nanoantennas with a rotational C3 symmetry are designed and characterized. The plasmonic nanoantennas are fabricated on top of the WS$_2$ monolayers and the optical properties are studied in the experiment.

O 48.4 Tue 18:15 Poster A

Structure and mechanical properties of carbon nanomembranes — •Florian Gayk, Julian Ehrens, Tjark Heitmann, Andreas Mrugalla, Patrick Vorndamme, and Jürgen Schnack — Universität Bielefeld, PF 100131, D-33615 Bielefeld

Carbon nanomembranes (CNMs) are successfully synthesised by irradiating monolayers of polyaromatic molecules with electrons which induces crosslinking [1]. But the internal structure of the resulting CNMs remains vague. To make a proposal we investigate them in terms of classical molecular dynamics calculations using LAMMPS. Since several classical carbon potentials are available we first study the accuracy of the potentials concerning Young's moduli by testing them on well known structures such as diamond or graphene. The second generation REBO and EDIP potentials turn out to provide reasonable results. We propose a method how to simulate the effect of the irradiation process in our molecular dynamics framework. The obtained CNM structures are discussed.

[1] P. Angelova et al., ACS Nano 7 (2013) 6489

O 48.5 Tue 18:15 Poster A

Electron Lattice Discretization in Two-Dimensional Hexagonal Flat Band Systems — •Maximilian Uhl[1,2] and Wolfgang Häusler[1] — [1]Institut für Physik, Universität Augsburg — [2]Present Adress: Max-Planck-Institut für Festkörperforschung, Stuttgart

The $\mathcal{T}_3$-lattice is a two-dimensional hexagonal lattice where jumps between certain lattice sites are suppressed by destructive quantum interference [2]. It features interesting properties such as a flat band where the electron single particle energies are constantly zero. Owing to Coulomb interactions, the electrons form Wigner crystals in the ground state. However, due to localization to specific lattice sites, perfect Wigner crystals can only be formed at commensurability with the underlying $\mathcal{T}_3$-lattice, requiring specific discrete electron densities [1]. Then, the system is insulating. At other electron densities, the extra carriers may contribute to a nonzero conductance [1]. The commensurability condition is described by an equation of integers [1]. At first glance, its distribution as a function of normalized electron density ν seems completely irregular. In this work, a twelvefold symmetry has been found, allowing for the identification of strong degeneracies. Analytical and numerical analysis revealed various unexpected properties such as that distances of commensurate ν^{-1} tend to be divisible by three or that the minimal distance of commensurate ν^{-1} always keeps appearing even for ν^{-1} going towards infinity.

[1] W. Häusler: Phys. Rev. B **91**, 041102 (2015)

[2] B. Sutherland: Phys. Rev. B **34**, 5208 (1986)

O 48.6 Tue 18:15 Poster A

Controlling the Topological Properties of Stanene: Realistic Modeling and Experimental Approaches for Substrates — •Maximilian Bauernfeind[1], Philipp Eck[2], Marius Will[1], Domenico Di Sante[2], Lenart Dudy[1], Ronny Thomale[2], Jörg Schäfer[1], Ralph Claessen[1], and Giorgio Sangiovanni[2] — [1]Physikalisches Institut and Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg

Stanene, the two-dimensional (2D) honeycomb lattice made of Sn atoms with its non-trivial topological electronic structure could play a revolutionary role in future electronic devices. A bottleneck to reach this ultimate goal is the fabrication of stanene on a substrate, without destroying its topological properties by strain or charge transfer, induced by the bonding situation. To overcome this problem, one approach is to decouple the stanene layer from the substrate. This may, e.g., be achieved by a buffer layer between the substrate and the stanene layer. We present a systematic study of buffer layers made of different group-III and group-V atoms on the wide-bandgap semiconductor SiC(0001). With band structure calculations based on density-functional theory (DFT), we observe a passivation of the SiC(0001) surface. Additionally, the buffer has an influence on the buckling and the vertical distance of the stanene layer. Some buffer layer materials render the stanene layer topological. First experimental data on the fabrication of an Al buffer layer will also be presented.

O 48.7 Tue 18:15 Poster A

Hexagonal Boron-Carbon-Nitrogen - a two-dimensional direct band gap semiconductor — •Axel Enders[1,3], Sumit Beniwal[2,3], Suchetana Sarkar[1], Paulo Costa[3], Peter Dowben[3], James Hooper[4], Daniel Miller[5], Eva Zurek[5], and Shih-Yuan Liu[6] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth — [2]Universität Erlangen-Nürnberg, 91058 Erlangen — [3]Dept. of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588, USA — [4]Dept. of Theoretical Chemistry, Jagellionian University, 30-060 Krakow, Poland — [5]Dept. of Chemistry, Buffalo, New York 14260, USA — [6]Dept. of Chemistry, Boston College, Chestnut Hill, MA 02467, USA

Two-dimensional h-BCN, synthesized from the precursor molecule bis-BN cyclohexane on the (111) surfaces of Ir and Rh under UHV, was investigated with a comprehensively suite of in-situ local probe microscopy and spectroscopy methods, combined with density functional theory. The lattice structure of h-BCN is identical to that of graphene, with the graphenic sites occupied by atoms of boron, nitrogen and carbon. On the basis of measured band gaps and the computationally predicted electronic band structure, especially a direct electronic band gap that is intermediate to those of the zero-band gap semiconductor graphene and the insulating h-BN, and the theoretical prediction that the band gap is dependent on the molecular tiling, it can be expected that the h-BCN layers are potentially exciting candidates for 2D electronic materials

O 48.8 Tue 18:15 Poster A

Effects of substrate on defects production in 2D inorganic materials under ion irradiation in Helium Ion Microscope — •Sadegh Ghaderzadeh[1], Silvan Kretschmer[1], Mikhail Maslov[1,2], Mahdi Ghorbani-Asl[1], and Arkady Krasheninnikov[1,3] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Moscow Institute of Physics and Technology, Dolgoprudny, Russia — [3]Department of Applied Physics, Aalto University School of Science, Finland

Helium Ion Microscope (HIM) does not only provide high-resolution images of the samples, but also creates the possibility of changing their morphologies in a controllable manner by introducing defects. Recently, two-dimensional (2D) materials including transition-metal dichalcogenides (TMDCs) have drawn attention as the promising building blocks for the future electronic devices. Exposure to energetic He ions has been shown to give rise to defect formation, but the mechanism of defect production in the TMDC samples on substrates is not fully understood. In this work, we study the effects of substrates on the creation of defects in 2D materials under He ion irradiation. Using a binary collision approach and analytical potential molecular dynamics, we show that while at low (less than 500 eV) He ion energies defects appear mostly due to direct ion impacts, at high energies defect creation is dominated by backscattered ions and atoms sputtered from the substrate. Our results provide microscopic insights into defect formation mechanisms in supported 2D materials.

O 48.9 Tue 18:15 Poster A

Time-resolved photoemission electron microscopy on monolayered WSe_2 — •Bernhard Huber[1], Sebastian Pres[1], Bernhard Mahlmeister[1], Daniel Fersch[1], Victor Lisinetskii[1], Steffen Michaelis de Vasconcellos[2], Robert Schneider[2], Johannes Kern[2], Matthias Hensen[1], Rudolf Bratschitsch[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Physikalisches Institut, Wilhelm-Klemm-Str. 10, 48149 Münster

Atomically thin transition metal dichalcogenides (TMDCs) have emerged as a promising material system for optoelectronic applications, e.g., as a single-photon source, which was recently demonstrated with a single layer of WSe_2 [1]. Here we present time-resolved photoemission electron microscopy (TR-PEEM) results on WSe_2 in a pump–probe spectroscopy scheme revealing spatio–temporal features at the 100 nm length scale. As illumination source a widely tunable high-repetition-rate (1 MHz) laser system pumping a non-collinear optical parametric amplifier is used, providing pulses from 900 nm down to 230 nm. In the presented experiment, a pump pulse centered at 700 nm excites slightly above the A exciton resonance (1.63 eV) which occurs at the K and K' points of the Brillouin zone. A probe pulse (350 nm) consequently transfers the excited-state manifold into photoemitted electrons which are detected with PEEM.

[1] J. Kern et al., Adv. Mater. **2016**, 28, 7101–7105

O 48.10 Tue 18:15 Poster A

Real time investigation of the growth of hexagonal boron nitride on metal surfaces using LEEM — •Miriam Raths[1,2], Janina Felter[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA)

The 2D material hexagonal boron nitride (hBN) has attracted strongest interest recently, due to its specific structural and electronic properties. As an insulator (band gap of >5eV) it is a very promising material for hetero-epitaxial systems in conjunction with other 2D materials. In this study, we aim for a deeper understanding of its nucleation and growth, as it is necessary to produce high quality monolayers of hBN. In-situ Low-Energy Electron Microscopy (LEEM) studies enable us to follow the formation of hBN monolayers on metal surfaces by chemical vapour deposition of borazine in real time. We report on the growth of hBN on the Ni(111) surface, and compare with earlier studies performed in our group on Cu(111) and Ag(111).

O 48.11 Tue 18:15 Poster A

Investigation of hybridized hexagonal boron nitride and graphene (hBNC) on SiC(0001) — •Shayan Parhizkar[1,2], Markus Franke[1,2], Serguei Soubatch[1,2], You-Ron Lin[1,2], Nafiseh Samiseresht[1,2], Miriam Raths[1,2], François C. Bocquet[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA-FIT)

Hybridized 2D heterostructures are of great interest due to their high variety of electronic properties and their great potential for future electronic and optoelectronic applications. Hexagonal boron nitride (hBN) and graphene, two well known 2D materials that are dielectric and conductive, respectively, have identical crystal structures and very similar lattice parameters. This makes them compatible in hybrid systems and motivates the investigation of their interaction.

Here we report on structural and electronic properties of hybridized hexagonal boron nitride and graphene (Gr-R0°), so-called hBNC, epitaxially grown on the wide bandgap semiconductor SiC as a function of the domain ratio. Starting from pure hBN to almost pure graphene, we investigated single 2D layers using X-ray standing waves (XSW) and (angular resolved) X-ray photoemission spectroscopy (ARPES and XPS).

O 48.12 Tue 18:15 Poster A

Growth and structure of mono- to few-layer vanadium disulphide on graphene on Ir(111) — •Joshua Hall[1], Tobias Wekking[1], Felix Huttmann[1], Stefan Kraus[1], Nico Rothenbach[2], Katharina Ollefs[2], Lucas M. Arruda[3], Nick Brookes[4], Gunnar Schönhoff[5], Jan Berges[5], Tim Wehling[5], Wolfgang Kuch[3], Heiko Wende[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [3]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [4]European Synchrotron Radiation Facility, ESRF, France — [5]Institut für Theoretische Physik, Bremen Center for Computational Materials Science, Universität Bremen, Germany

Using scanning tunnelling microscopy and low-energy electron diffraction we study the growth and structure of vanadium disulphide VS$_2$. The mono- to few-layer samples of VS$_2$ on graphene on Ir(111) are grown by in situ molecular beam epitaxy. Depending on the specific growth parameters, a variety of growth scenarios evolves. Monolayer VS$_2$ displays smoothly joined domains of a (3×1) superstructure that appears to result from an uniaxial distortion and buckling of the hexagonal VS$_2$ lattice. In X-ray circular magnetic dichroism experiments, the ferromagnetism proposed in monolayer VS$_2$ [1] is not found. In few-layer VS$_2$, the hexagonal lattice is restored, still exhibiting multiple superstructures.

[1] Isaacs and Marianetti, PRB 94, 035120 (2016)

O 48.13 Tue 18:15 Poster A

Vibronic spectroscopy of single phthalocyanine molecule on MoS$_2$/Au(111) — •Gaël Reecht, Nils Krane, Christian Lotze, and Katharina J Franke — Freie Universität Berlin , Berlin ,Germany

Transition metal dichalcogenides (TMDC) as MoS$_2$ are two-dimensional semiconducting materials. Single layer TMDC are particularly promising as they present a direct band-gap at the K point, a giant excitonic renormalization and a spin splitting of the valence band. Due to the presence of a band gap, MoS2 can also be used to decouple nanostructures from a metallic substrate. With a LT-STM, we studied phthalocyanine molecules (Zn-Pc and H$_2$-Pc) on MoS$_2$ grown previously on Au(111). As reported for other decoupling systems (graphene, NaCl, H-BN), we observe a high spatial resolution of the molecular orbitals on MoS$_2$. Moreover, for the molecular states with an energy in the gap of MoS$_2$, the lifetime of the state is strongly enhanced and a series of vibronic modes can be resolved. In the extreme case of the H$_2$-Pc, vibronic states with energies from few meV to hundreds of meV are observed. Finally, we compare the measured vibrational energies with results of DFT, Raman spectroscopy and LE-STM.

O 48.14 Tue 18:15 Poster A

Li Adatoms on Single Layer Molybdenum Disulfide on Au(111) — •Asieh Yousofnejad, Timo Kubsch, Nils Krane, Gaël Reecht, Christian Lotze, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin

Two-dimensional transition metal dichalcogenides (2D TMDCs) have attracted attention recently because of their interesting electronic and optical properties. Molybdenum disulfide (MoS$_2$) shows a transition from an indirect band gap in bulk structure to a direct band gap in the monolayer structure. In order to obtain functional devices, tuning of the band structure is desirable. One approach to achieve this is for instance doping by alkali atoms.

Here, we grow MoS$_2$ on Au(111) by depositing Mo and annealing in an H$_2$S atmosphere. We then deposit Li on a sample at a temperature below 110K. We observe single Li atoms on the MoS$_2$ islands. However, at measuring temperatures of 4K these atoms are mobile and can be easily dragged by the STM tip. Using Scanning Tunneling Spectroscopy we do not find evidence for a change of the band gap of MoS$_2$, suggesting a negligible charge transfer.

O 48.15 Tue 18:15 Poster A

Intra- and inter-layer magnetic interactions in a van der Waals crystal — •Moemi Kawashima[1,2], Akira Akaishi[2], and Jun Nakamura[2] — [1]Department of Engineering Science, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan — [2]Institute of Condensed Matter Theory and Optics, Jena, Germany

Chromium triiodide (CrI$_3$) with a layered structure is known to be a soft ferromagnet in its bulk form. Huang *et al.* recently reported that the magnetic properties of CrI$_3$ differ when the layers approach the 2D limit, and become sensitive to the number of layers: monolayered and trilayered CrI$_3$ are ferromagnetic, whereas bilayered CrI$_3$ happens to be antiferromagnetic. In order to explore the mechanism of such a layer-number dependent magnetism of CrI$_3$, we have investigated the magnetic properties of CrI$_3$ thin films using the van der Waals density functional theory. We have found out that the ground states for all of monolayered, bilayered and trilayered CrI$_3$ are ferromagnetic, in both the low-temperature (R$_{\overline{3}}$ with an ABC-stacking) and high-temperature (C$_{2/m}$ with another ABC-stacking) structure. However, it has been revealed that trilayered CrI$_3$ is most stable with an AA-stacked structure, and the magnetic ground state of bilayered CrI$_3$ becomes antiferromagnetic with an AA-stacked structure. These results suggest that the bilayered CrI$_3$ observed in the experiments of Huang *et al.* had an AA-stacked structure, and that the crystallographic properties of 2D CrI$_3$ have a strong connection to its magnetism. We will also discuss impacts of the choice of the van der Waals functional on the magnetic interaction through van der Waals interactions.

O 48.16 Tue 18:15 Poster A

Photoemission electron microscopy study of MXene microflakes — •Bharti Parashar[1], Pika Gospodaric[1], Kanit Hantanasirisakul[2], Slavo Nemsak[1], Tomas Duchon[3], Johanna Hackl[1], Lukasz Plucinski[1], Steven May[2], Yury Gogotsi[2], and Claus M. Schneider[1] — [1]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Drexel University Materials Science & Engineering, 3141 Chestnut Street (LeBow 344), Philadelphia, PA 19104 U.S.A. — [3]Department of Surface and Plasma Science, Charles University in Prague, Czech Republic

Recent advances in photoemission electron microscopy (PEEM) facilitate access to electronic structure with sub-100 nm lateral resolution, either through x-ray absorption (XAS) or photoemission (PES) spectroscopy. Utilizing these techniques, we have studied thin chemically exfoliated Ti$_3$C$_2$ MXene microflakes prepared on Si(001) and HOPG substrates. Well-separated single flakes of approx. 5 micrometers in size were characterized with respect to their functionalization with F$^-$, OH$^-$, and O^{2-} groups. The results revealed fluorine-rich clusters of up to 1 micrometer in diameter distributed non-uniformly on the surface of the flakes and we observed their influence on the electronic structure of Ti.

These results provide important complementary information to other, spatially non-resolved techniques, and they are the first steps towards understanding of the electronic band structure of these microscopic objects.

O 48.17 Tue 18:15 Poster A

Interaction of slow highly charged ions with 2D materials — •Sascha Creutzburg[1], Janine Schwestka[2], Tibor Lehnert[3], Robert Leiter[3], Arkady V. Krasheninnikov[1], Roland Kozubek[4], René Heller[1], Stefan Facsko[1], Ute Kaiser[3], Marika Schleberger[4], Friedrich Aumayr[2], and Richard A. Wilhelm[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research — [2]TU Wien, Institute of Applied Physics — [3]Ulm University, Central Facility of Electron Microscopy — [4]University Duisburg-Essen, Faculty of Physics and CENIDE

The neutralisation of highly charged ions (HCIs) upon impact on a solid surface occurs within a timescale smaller than about 10 fs [1,2]. Recently, freestanding 2D layers became available and their utilization for transmission studies of HCIs makes a more detailed investigation of the neutralisation mechanisms possible. The charge exchange of HCIs transmitted through single layer graphene [1] and carbon nanomembranes [3] was investigated by means of an electrostatic analyser. Additionally, the ion stopping is measured and the kinetic energy loss depends strongly on charge exchange. In this contribution the transmission measurements are extended to 2D materials beyond graphene, i.e. MoS$_2$ and hBN.

[1] E. Gruber et al., Nat. Commun. 7, 13948 (2016).
[2] R. A. Wilhelm et al., Phys. Rev. Lett. 119, 103401 (2017).
[3] R. A. Wilhelm et al., Phys. Rev. Lett. 112, 153201 (2014).

O 48.18 Tue 18:15 Poster A

Ellipsometric determination of the anisotropic refractive index of WSe$_2$ via angle resolved measurements for E = 1.89 eV — •Walter Enns[1], Sergej Neb[1], Sebastian Fiechter[2], and Walter Pfeiffer[1] — [1]Universität Bielefeld, Fakultät für Physik, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Helmholtz Zentrum Berlin, Institut für Solare Brennstoffe, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Although the transition metal dichalcogenide (TMDC) van der Waals crystals are obviously optically anisotropic, little information is found in literature. Experimental determination of the optical anisotropic response is complicated by the preferential cleaving of crystals along the van der Waals gaps. In addition the formation of a contamination layer in air and the macroscopicly uneven surface are further experimental hurdles. Here it is shown that precise angle resolved ellipsometric single-wavelength measurements combined with statistical and error analysis enables extracting the complex anisotropic refractive index from the coupled ellipsometric values Δ and Ψ. The experimentally obtained values show reasonable agreement with theoretical calculations of the dielectric function [1, 2].

[1] S. Sharma, et al., Phys. Rev. B **60**, 8610 (1999)

[2] A. Kumar, et al., Physica B: Condensed Matter **407**, 24 (2012)

O 48.19 Tue 18:15 Poster A

Hot carrier dynamics in semiconducting transition-metal dichalcogenides – valley-polarized excitation in bulk $2H$-MoS$_2$ and monolayer WS$_2$/Au(111) — •Hauke Beyer[1], Gerald Rohde[1], Antonija Grubisic Cabo[2], Ankatrin Stange[1], Luca Bignardi[3], Daniel Lizzit[3], Paolo Lacovig[3], Silvano Lizzit[3], Kai Rossnagel[1], Philip Hofmann[2], and Michael Bauer[1] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [3]Elettra Sincrotrone Trieste, S.S. 14 Km 163.5, 34149 Trieste, Italy

Time- and angle-resolved photoelectron spectroscopy (trARPES) is employed to study the valley-selective excitation and near-surface dynamics of carriers at K and K′ in semiconducting transition-metal dichalcogenides (TMDC). Upon photoexcitation with circularly polarized laser pulses ($\lambda \approx 600\,\mathrm{nm}$), circular dichroism can be observed in excited-state intensity as well as dynamics. The poster will present and compare experimental results of bulk $2H$-MoS$_2$ and monolayer WS$_2$/Au(111). In the latter case, we observe a significantly enhanced dichroism of the excitation intensity in comparison to the bulk sample, which we attribute to the lack of mirror domains of the WS$_2$ sample. Furthermore, a dependence of the population dynamics on the polarization state of the excitation laser pulse is observed only for $2H$-MoS$_2$. This difference is associated with K to K′ intervalley scattering processes affecting the carrier dynamics in bulk TMDC samples but being absent in the case of monolayer WS$_2$/Au(111).

O 48.20 Tue 18:15 Poster A

Tuning optoelectronic properties on 2D material devices — •Nieves Morquillas[1], Saül Veléz[1,3], Felix Casanova[1,2], Luis Hueso[1,2], Reyes Calvo[1,2], and Jose Ignacio Pascual[1,2] — [1]CIC nanoGUNE, 20018 San Sebastian (Spain) — [2]Ikerbasque, 48011 Bilbao (Spain) — [3]Department of Materials, ETH Zürich, 8093 Zürich (Switzerland)

Transition metal dichalcogenides are promising materials for optoelectronis due to their tunability. We characterize the optoelectronic properties of semiconducting 2D devices by combined photoluminescence and electric transport measurements in a scanning photocurrent microscope (SPCM). We study the photocurrent created at Schottky barriers of MoS2 devices, including systems with an interface between 1L and 2L showing a potential barrier at the boundary. We also investigated a heterostructure of MoS2 on top of NbSe2, a strong electron acceptor, where we find areas at the heterostructure with a high on/off current ratio.

Another tunable property is the pseudo-spin. For an odd number of layers, inversion symmetry is broken and thus it is possible to tune a new degree of freedom, the valley. Here we investigate the effect of a ferrimagnetic substrate (Yttrium Iron Garnet, YIG) on the pseudo-spin of a WSe2 single layer by circularly polarized light in a scanning confocal microscope (SCFM). The ferrimagnetic substrate has a characteristic magnetic domain arrangement with an effective out-of-plane magnetic field. Contrary to expected, we observed a stronger effect from the substrate roughness than from the effective magnetic field.

O 48.21 Tue 18:15 Poster A

Magnetic Field Dependence of Energy Dissipation on a Topological Insulator Surface Studied by Pendulum AFM — •Dilek Yildiz[1,2], Marcin Kisiel[1,2], Urs Gysin[1], and Ernst Meyer[1] — [1]Universität Basel, Department of Physics, Basel, Switzerland — [2]Swiss Nanoscience Institute, Basel, Switzerland

Bodies in relative motion separated by few nanometers gap experience 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. Such frictional nature on layered systems is yet another exotic playground. Topological insulators, such as Bi2Te3 present an opportunity to investigate multiple facets of non-contact friction. Although electronic properties of topological insulators have been studied extensively, frictional response of those surfaces are yet to be reported. We studied energy dissipation on Bi2Te3 surface by means of pendulum geometry AFM/STM. Energy dissipation peaks were measured few nanometers above the surface at relatively large voltages. Such dissipation peaks are observed to shift as a function of external magnetic field. Our results indicate that energy dissipation is mainly due to electrostatic friction.

O 49: Poster: Nanostructures on Surfaces I

Time: Tuesday 18:15–20:30 Location: Poster A

O 49.1 Tue 18:15 Poster A

Ullmann Coupling of 1,3-Dibromoazulene — •Claudio K. Krug, Qitang Fan, Florian Fillsack, Johannes Glowatzki, Nicole Trebel, Martin Schmid, and J. Michael Gottfried — Department of Chemistry, Philipps-Universität Marburg, Germany, Hans-Meerwein-Str. 4, 35032 Marburg

The surface-confined Ullmann coupling reaction is a well-established strategy for creating covalent bonds between formerly halogenated aromatic molecules on coinage metal surfaces. So far, the focus has been on benzoid carbon backbones with alternant topologies. Here, we report the first Ullmann coupling involving a non-alternant aromatic hydrocarbon backbone. Specifically, the reaction of 1,3-dibromoazulene (DBAz) on Cu(111) was studied by means of scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) under ultrahigh vacuum (UHV) conditions. Upon room temperature deposition of DBAz on Cu(111), long regioirregular chains are formed. The organometallic character suggested by the lattice constant is confirmed by XPS. Annealing to 440 K transforms the chains to cyclic organometallic hexamers with high yield. We have investigated the formation of these hexamers depending on the surface coverage. At low coverages, only isolated hexamers are observed because of lateral repulsive interactions. Increasing the coverage yields larger islands of Cu-DBAz cyclic hexamers. Annealing to higher temperatures results in the formation of regioregular covalent chains.

O 49.2 Tue 18:15 Poster A

Vibrational eigenmodes of the Sn-($\sqrt{3}\times\sqrt{3}$)/Si(111) reconstruction observed by surface Raman spectroscopy — •Benedikt Halbig, Utz Bass, and Jean Geurts — Universität Würzburg, Experimentelle Physik III, Würzburg, Germany

Adatoms on semiconductor surfaces, like Si(111), may reconstruct as two-dimensional layers leading to novel properties. For our subject Sn-($\sqrt{3}\times\sqrt{3}$)/Si(111), effects like a row-wise antiferromagnetic spin ordering [1] and a temperature-induced metal-insulator-transition were reported, but no phase transition [2,3]. Structure determination via surface sensitive Raman spectroscopy was successfully shown for surface adlayers [4].

We report on polarization dependent *in situ* Raman spectra of Sn-($\sqrt{3}\times\sqrt{3}$)R30°/Si(111) at 300 K and ≈ 20 K. In contrast to the unreconstructed surface, new Raman peaks arise, the strongest ones at 184 and 383 cm^{-1}. Upon sample cooling, no significant changes in the Raman spectra were observed. In accordance with literature, we therefore acknowledge no phase transition.

In particular we observe a theoretically predicted mode at 81 cm^{-1} [3]. Unlike in the reports for Sn/Ge(111), this mode is not softening with decreasing temperature and not responsible for a change of the surface reconstruction, in agreement with theory prediction for Sn/Si(111) [3].

[1] G. Li et al., nat. comm. **4**, 1620 (2013) [2] S. Modesti et al., PRL **98**, 126401 (2007) [3] R. Pérez et al., PRL **86**, 21 (2001) [4] M.

Liebhaber et al., PRB **94**, 235304 (2016).

O 49.3 Tue 18:15 Poster A

Self-assembly & optoelectronic properties of bis- & tetra-pyridil functionalized pyrene molecules — •Domenik Zimmermann[1], Knud Seufert[1], Luca Dordevic[2], Tomas Marangoni[2], Davide Bonifazi[3], and Willi Auwärter[1] — [1]Physik-Department E20, Technische Universität München, Germany — [2]Department of Chemical and Pharmaceutical Sciences, University of Trieste, Italy — [3]Department of Chemical and Pharmaceutical Sciences, University of Trieste, Italy

Pyridil functionalized pyrenes have shown well defined self-assembled structures on Ag(111). Dependent on the number and geometric positioning of the substituents, one-dimensional coordination chains, two-dimensional arrays and chiral, porous kagomé-type networks have been tailored in UHV and were investigated by STM[1].

However, to address the photoactivity of these polycyclic aromatic hydrocarbons an electronic decoupling from the metallic support is mandatory and achieved here by using an insulating layer of h-BN on Cu(111)[2]. On this electronically nanopatterned but topographically weakly corrugated substrate the molecules form self-assemblies reminiscent of the Ag case but show a distinct band gap between prominent HOMO/LUMO states. STS shows a decrease of this gap upon increasing the number of substituents of the pyrene core. This result is confirmed by gas phase DFT calculations and UV-Vis spectra in solution.

[1] Kaposi et al, ACSNano **10**, 7665 (2016)
[2] Joshi et al, Nano Letters **12**, 5821 (2012)

O 49.4 Tue 18:15 Poster A

Efficient anchoring of molecular end groups via electric field driven chemical reaction — •Tomasz Michnowicz[1], Bogdana Borca[1,2], Remi Petuya[3], Marcel Pristl[1], Verena Schendel[1], Ivan Pentegov[1], Ulrike Kraft[1], Hagen Klauk[1], Peter Wahl[1,4], Andres Arnau[3,5], Uta Schlickum[1], and Klaus Kern[1,6] — [1]Max Planck Institute for Solid State Research, Germany — [2]National Institute of Materials Physics, Romania — [3]Donostia International Physics Centre, Spain — [4]Unviersity of St Andrews, United Kingdom — [5]Basque Country University CSIC-UPV/EHU, Spain — [6]Ecole Polytechnique Federale de Lausanne, Switzerland

One of the challenges of single molecule electronics is to form a stable bond of the desired molecule to the metal electrodes, providing low resistance at the molecule-metal interfaces. One of the tools allowing both controlled manipulation of single molecules and probing their properties, including the electric conductance, is Scanning Tunnelling Microscopy (STM). We show that a direct desulfurization reaction of a single thiophene unit embedded in a tetracenothiophene molecule on a Cu (111) surface can be driven by an electric field present in the STM tip-sample junction. This controlled, atomically precise reaction leads to the formation of covalent bonds between two carbon and two copper surface atoms. The enhanced coupling leads to 50% increase of the electric conductance measured by precisely contacting the molecules at the desired atomic positions and forming a molecular bridge between the metallic STM tip electrode and the metallic surface electrode.

O 49.5 Tue 18:15 Poster A

2D Nanoporous Chiral Supramolecular Networks Steered by Two σ-hole Interactions of S-Br & Br-Br. — •Lingbo Xing[1], Zhichao Huang[1], Jingxin Dai[1], Zhaohui Wang[2], and Kai Wu[1] — [1]College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China — [2]Key Laboratory of Organic Solid, Chinese Academy of Sciences, Beijing 100190, China.

A variety of weak interactions such as hydrogen bonds, dipole-dipole interactions, van der Waals interactions, and metal-ligand coordination have been employed to assemble 2D nanoporous supramolecular networks at surfaces. σ-hole bond is a noncovalent interaction between a covalently-bonded atom of Groups IV-VII and a negative site, e.g. a lone pair of a Lewis base or an anion. Halogen bonding is a subset of σ-hole interactions. In this study, self-assembly behaviors of 3,10-dibromo-perylo[1,12-b,c,d]thiophene (2BPET) on Ag(111) will be discussed by means of scanning tunneling microscopy (STM) and density functional theory (DFT) calculations. For the first time, S-Br σ-hole interactions act as the driven force of molecular assembly on metal surfaces. Three types of porous chiral assembly phases can be fabricated under different coverage and deposition temperature steered by S-Br and Br-Br. Combined with DFT calculations, it turns out that S-Br is more thermodynamic stable.

O 49.6 Tue 18:15 Poster A

A Family of Hierarchical Molecular Fractal Porous Networks Constructed by a Small Molecule at Surface — •Jingxin Dai, Jian Shang, Wenhui Zhao, Lingbo Xing, and Kai Wu — SKLSCUSS, BNLMS, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.

By using B3PB as the precursor, standalone molecular fractals (Sierpiński triangles, ST-n, n = 0, 1, 2, 3, 4, etc.) consisting of B3PB were constructed on Ag(111). The B3PB-ST-n fractals further formed new building motifs that self-assembled into a whole series of hierarchical two-dimensional molecular networks via a unified assembling pattern (rhombus unit cell containing two opposite chiral structures of the ST-n series). This unique hierarchical molecular self-assembly involved both fractal features and hierarchical features at the same time, and could provide new possibilities towards novel and complex hierarchical assemblies.

O 49.7 Tue 18:15 Poster A

Adsorption and Assembly of Photoelectronic TiOPc Molecules on Coinage Metal Surfaces — •Wenhui Zhao, Hao Zhu, and Kai Wu — College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China

The adsorption and assembly of individual and sub-monolayered TiOPc on Ag(111), Cu(111) and Au(111) has been investigated by STM and STS. High-resolution STM imaging and dI/dV and I - z measurements reveal that TiOPc adsorbed on Ag(111) possesses two configurations, i.e., O-up and O-down configurations. Dipole-dipole interactions drive the TiOPc molecules to form a highly ordered checkerboard assembly structure on Ag(111) with alternating rows of the O-up and O-down adsorption conformations. The restricted surface mobility and diffusivity due to the strong interaction between the Cu(111) substrate and the TiOPc molecules and the templating effect of the reconstructed Au(111) herringbone structure result in no assemblies of the TiOPc molecules on these surfaces. Instead, the experimentally observed molecular dimers on both Au(111) and Cu(111) as well as the molecular aggregates on Au(111) indicate that the intermolecular dipole-dipole attraction and weak hydrogen bonding play an important role in dictating the adsorption and steering the assembly of the TiOPc molecules on the coinage metal surfaces.

O 49.8 Tue 18:15 Poster A

Hong-Ou-Mandel interference on dielectric metasurfaces — •Philip Christian Georgi[1], Kai Hong Luo[1], Fabian Meyer[1], Guixin Li[2], Christine Silberhorn[1], and Thomas Zentgraf[1] — [1]University of Paderborn, Paderborn, Germany — [2]Southern University of Science and Technology, Shenzhen, China

Metasurfaces enable a spatial phase and amplitude manipulation of light, which makes them a powerful and versatile tool for all kinds of optical applications, especially holography. In contrast to their plasmonic counterparts, dielectric metasurfaces are inherently lossless and in recent years they gained an increased popularity in the research community due to the achievement of high operational efficiencies. This property makes them interesting for quantum optical application. As an initial step in this direction we present a recreation of the Hong-Ou-Mandel experiment based on a dielectric metasurface.

O 49.9 Tue 18:15 Poster A

2D self-assembly of TPT on noble metal surfaces — •Sebastian Becker[1,2], Lu Lyu[1], Sina Mousavion[1], Maniraj Mahalingam[1], Markus Gerhards[2], Benjamin Stadtmüller[1,3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern — [2]Department of Chemistry, University of Kaiserslautern, Erwin-Schrödinger-Str. 52, 67663 Kaiserslautern — [3]Graduate School Materials Science in Mainz, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

Interfacial properties of organic films on noble metal surfaces are determined by a delicate balance between different interactions at the interface. Here, we investigate the geometric and electronic structures of TPT (2,4,6-triphenyl-1,3,5-triazine) on three (111) different noble metal surfaces with different surface reactivity using LT-STM and LEED. On Cu(111), TPT forms a long range ordered honeycomb-like metal-organic network with Cu adatoms in which the nitrogen atoms of the triazine ring adsorb on top of the Cu atoms[1]. In contrast, a close packed herringbone structure is observed for TPT on the less reactive Ag(111) and Au(111) surfaces at RT. Most interestingly, for TPT/Ag(111), we find a temperature-driven structural phase transition from the herringbone structure at RT to a honeycomb-like cavity structure at LT which was not observed for the other surfaces. Our findings will be correlated to the surface reactivity and the corresponding molecule-substrate interaction of each adsorbate system. [1] PRB 95, 094409 (2017)

O 49.10 Tue 18:15 Poster A

Formation of Metal-Organic Coordination Networks on a Bulk Insulator Surface — •Lukas Schüller[1], Md Taibur Rahman[1], Ralf Bechstein[1], and Angelika Kühnle[2] — [1]Institute of Physical Chemistry, Johannes Gutenberg University Mainz, Duesbergweg 10-14, 55128 Mainz, Germany — [2]Department of Chemistry, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany

Metal-organic coordination networks (MOCNs) are a class of two-dimensional compounds with potentially interesting electronic, magnetic and catalytic properties. A variety of MOCNs have been created on metal surfaces. However, an underlying insulator surface is beneficial for the electronic decoupling of structure and surface. To this end, we demonstrate the self-assembly of organic linker molecules and the formation of MOCN precursor structures in the presence of iron nanoclusters at room temperature. Our study of biphenyl-4,4'-dicarboxylic acid (BPDCA) in presence of iron on calcite (10.4) unravels two important findings: First, the deposition order plays a vital role in the formation of MOCNs. Second, a strong templating effect of the underlying surface is decisive for the direction, in which the MOCN is more extended. Currently, we vary the size of the linker molecule in order to match the surface unit cell size. Terephtalic acid (TPA), a homologue of BPDCA with one phenyl ring less, is examined in presence of iron, as well as 1,1':4',1"-terphenyl-4,4"-dicarboxylic acid (TPDCA), i.e., the homologue of BPDCA with one phenyl ring more. With this work, we explore the formation of an extended MOCN on an application-relevant bulk insulator surface.

O 49.11 Tue 18:15 Poster A

Simulation of reversibly interlocked SWCNTs — •Sebastian Gsänger and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

In chemical functionalization of single-walled carbon nanotubes (SWCNTs), usually one has to compromise between altering the structure of the nanotube via covalent attachment of the adsorbates or by forming rather fragile supramolecular complexes. An alternative, which combines having only non-covalently bound species but leads to very stable structures, is the concept of mechanically interlocking the CNT inside the adsorbate molecule. Specifically, we explore adsorbates which allow for a reversible ring closure in the rotaxane-forming step, therefore promising greater yields and a better control of the target structure. By combining classical molecular dynamics with DFT and metadynamics in a QM/MM approach we shed light on the adsorption behavior and the ring-closure reaction in different environments.

O 49.12 Tue 18:15 Poster A

Radiation pattern of the third harmonic emission generated in metal nanoantennas — •Torsten Stiehm, Johannes Kern, Robert Schmidt, Marius Jürgensen, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics and Center for Nanotechnology University of Münster, 48149 Münster, Germany

Plasmon resonances in metallic nanoantennas give rise to strong field enhancements. This drastically boosts the nonlinear light-matter interaction in the metal and enables efficient third harmonic generation. We measure the angular distribution of the third harmonic emission of gold nanoantennas [1]. Single and multiple nanoantennas with resonances in the infrared [2] are excited by ultrashort laser pulses. The third harmonic emission is analyzed with back focal plane imaging using a high numerical aperture objective lens. Our experimental findings are in excellent agreement with numerical calculations.

1. T. Stiehm, J. Kern, M. Jürgensen, S.M. de Vasconcellos, R. Bratschitsch, Appl. Phys. B 122, 1 (2016)

2. T.Stiehm, J.Kern, R.Schmidt, S.M. de Vasconcellos, R. Bratschitsch, Appl. Phys. B 123, 150 (2017)

O 49.13 Tue 18:15 Poster A

Material sensitive reconstruction of nanostructures based on finite-element simulations of complementary X-rays measurements — •Victor Soltwisch, Analia Fernandez Herrero, Philipp Hönicke, Mika Pflüger, Burkhard Beckhoff, and Frank Scholze — Physikalisch-Technische Bundesanstalt, Berlin

In order to model visible light scattering, rigorous calculations of the near and far field by numerically solving Maxwell's equations with a finite-element method are well established. The application of this technique to X-rays is still challenging, due to the discrepancy between the incident wavelength and the discretization size. We show that a rigorous calculation of the near and far field is still suitable for grazing incidence techniques e.g. grazing incidence small angle X-ray scattering (GISAXS) or grazing incidence X-ray fluorescence (GIXRF) and 2D periodic nanostructured surfaces. The flexibility of the finite-element approach in combination with statistical evaluations allows for parameter reconstruction of the surface shape with sub-nm uncertainty. This combined toolset of scattering and fluorescence measurements with rigorous simulations paves the way for a versatile characterization of nanoscale structured surfaces.

O 49.14 Tue 18:15 Poster A

Reactivity of CO on Sulfur-Passivated Graphene-Supported Platinum Nanocluster Arrays — Fabian Düll, Udo Bauer, Florian Späth, Philipp Bachmann, Johann Steinhauer, Hans-Peter Steinrück, and •Christian Papp — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

Poisoning of heterogeneous catalysts, in particular platinum, by sulfur and its oxides is of a hot topic in catalysis for decades.

Utilizing the intrinsic Moiré pattern of graphene on Rh(111) as a template and chemically inert support, Pt nanocluster arrays were grown.[1] They were then poisoned with sulfur via thermal reduction of SO2. To understand the changes that occur upon sulfur poisoning, the adsorption and desorption of the probe molecule CO were investigated. The changes in the adsorption behavior for several preadsorbed sulfur coverages were studied with in situ high-resolution XPS. Three different CO species can be distinguished: top and bridge bonded CO on terrace sites and CO at step sites. Sulfur blocks those adsorption sites to different degrees. While on-top and step sites are highly affected, bridge sites are affected to a lower degree. These results will be compared to measurements on the stepped Pt(322) and Pt(355) surfaces.[2] Upon annealing, a displacement of sulfur from step to terrace sites by CO occurs around 330 K, which is reversed after desorption of the CO. Such a behavior was also found on stepped platinum crystals.

[1] K. Gotterbarm et al., ACS Catal. (2015) 2397-2403.

[2] R. Streber et al., Chem. Phys. Lett. 452 (2008) 94-98.

O 49.15 Tue 18:15 Poster A

Studying surface interactions of molecular polyoxovanadate species for new electronic nanodevices — •Marco Moors[1], Oliver Linnenberg[2], Maria Glöss[1,2], Aleksandar Kondinski[2], and Kirill Monakhov[1,2] — [1]Forschungszentrum Jülich — [2]RWTH Aachen

Polyoxovanadates (POVs) have already been for a long time in the focus of several experimental and theoretical studies due to their synthetic accessibility, versatile structural chemistry, and intriguing electronic and magnetic properties. The possible applications for POVs cover many different fields of interest ranging from catalysis to nanoelectronics. A very promising approach is hereby their implementation as redox active centers in resistive switching memory cells. However, one of the most important challenges for a technological integration of such molecular systems in real devices is the controlled deposition of single POVs on surfaces and their individual contacting.

In our recent study we investigate the deposition of [V18O42I]5- on Au(111) by droplet deposition from different solvents and by thermal deposition from the solid phase. This mixed-valent superkeggin-type POV is a perfect candidate for molecular switching experiments due to its several and easily addressable vanadium redox states. Depending on the deposition technique and parameters we are able to control the particle size on the surface ranging from small agglomerates over single molecules up to molecular fragments, which tend to recombine on the metallic substrate leading to new low-valent vanadium-oxo species.

O 49.16 Tue 18:15 Poster A

Silver clusters in ionic liquids of different viscosity - stabilisation and aggregation — •Philippe Poulet, Florian Lippert, Alexander Kononov, Stefanie Roese, and Heinz Hövel — Fakultät Physik/DELTA, Technische Universität Dortmund, 44227

Dortmund, Germany

Due to their low vapor-pressure, enabling cluster deposition to liquids, Ionic Liquids (IL) gained interest for vacuum application [1]. Due to the relativly high viscosity of the IL at low temperature the aggregation of deposited clusters is significantly slowed down and the clusters stay separated. However, during cluster deposition a high viscosity hinders the mixing of the clusters into the volume of the IL.

For ILs with high viscosity Ag-clusters are deposited by temperatures higher than room-temperature to decrease the viscosity of the ILs and the temperature is decreased afterwards for storage. Via UV/vis-spectroscopy the aggregation of clusters is measured in-situ and ex-situ for different storage-temperatures.

Therefore the refractive indices depending on the wavelength are measured via Fabry-Pérot-Interferometry for the ILs [BMIM] [PF$_6$], [BMIM] [BF$_4$], [BMIM] [TF$_2$N], [BMIM] [DCA], [OMIM] [BF$_6$] and [EMIM] [FAP].

Additionally the temperatures for the glass transition of the above mentioned ILs are determined by measuring transmission.

[1] D. C. Engemann, S. Roese, H. Hövel, J. Phys. Chem. C **120**, 6239, (2016)

O 49.17 Tue 18:15 Poster A

Chemical Analysis of engineered Nanomaterials using Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) — •Markus Rennhak, Thomas Heinrich, and Wolfgang E. S. Unger — Bundesanstalt für Materialforschung und -prüfung, Fachbereich 6.1 Oberflächenanalytik und Grenzflächenchemie, Unter den Eichen 87, 12205 Berlin

The analysis of nanomaterials is current an important task - especially in case of risk assessment, as the properties of these material class are not well understood currently. The rather high surface area of these objects renders their interactions significantly different to their corresponding bulk. Thus, the surfaces chemical composition has to be investigated to get a better understanding and prediction of the nanomaterials' behavior. ToF-SIMS has proven as a powerful tool to determine said chemical composition. Its superior surface sensitivity allows us to study mainly the utmost atomic layer and therefore gives us an idea of the interactions involved. Here, we show first result from the validation of the method for the analysis of polystyrene and gold nanoparticles. ToF-SIMS will be compared to other methods like XPS, T-SEM or REM. Furthermore, principle component analysis (PCA) will be used to detect the influence of different sample preparation performed by an innovative microfluidic device. ToF-SIMS imaging is desired to be implemented for single particle detection as well.

O 49.18 Tue 18:15 Poster A

Temperature-dependent stabilization of silver nanoparticles in BMIM PF$_6$ — •Stefanie Roese, Alexander Kononov, Florian Lippert, and Heinz Hövel — Technische Universität Dortmund, Dortmund, Germany

The storage of nanoparticles(NPs) is one of the most challenging tasks. It is indispensable to prevent the NPs from aggregation to larger agglomerates after production. Many groups report that the NPs are electrosterically stabilized without additional agents by ionic liquids(ILs). A detailed review is given by Dupont and Scholten[1]. In addition, due to their low vapour pressure, ILs are ideally suited for vacuum applications. We investigated the temperature-dependent aggregation of preformed 2 nm silver NPs, which were produced by supersonic nozzle expansion and were deposited in a BMIM PF$_6$ IL[2]. With the help of the UV/VIS spectroscopy measurements and the analysis of the theoretically calculated spectra based on the Generalized Mie Theory for various shapes of aggregates, we were able to explain the stability of the samples with the temperature dependence of the viscosity of BMIM PF$_6$[3]. The same approach was also applied to samples produced by sputtering, to investigate the aggregation process. In this case the size distribution of the NPs is not fixed, as the formation of NPs by sputtering is likely to occur on the surface or in the first layer of the IL during and after the sputter deposition. [1] J. Dupont, J. D. Scholten, Chem. Soc. Rev. **39**, 1780, (2010). [2] D. C. Engemann, S. Roese, H. Hövel, J. Phys. Chem. **120**, 6239, (2016). [3] S. Roese, A. Kononov, J. Timoshenko, A. I. Frenkel, H. Hövel, submitted (2017).

O 49.19 Tue 18:15 Poster A

Topographic and Phase Measurements of Embedded Gold Nanoparticles using Atomic Force Microscopy — •Annika Bergmann, Sven Kraft, Regina Lange, Sylvia Speller, and Ingo Barke — University of Rostock, Institute of Physics, 18059 Rostock, Germany

For functional mapping of nanoscale samples a clear distinction between topographic effects and the signal of interest is inevitable. In atomic force microscopy (AFM) phase images do not only reveal material contrast but they may also contain topographic information [1], which is sometimes referred to as topographic crosstalk. Here we study the phase contrast between gold-nanoparticles and a PMMA environment using AFM. In order to obtain largely "pure" phase images we aim at creating a planar surface by embedding the nanoparticles into the polymer matrix. To achieve this, two different approaches are taken: first, heating of the sample which enables the nanoparticles to sink into the PMMA layer [2]; and secondly, spin-coating an additional PMMA layer on top of the sample. Our results show phase contrasts which have been detected for both approaches. Residual topographic effects are discussed, as well as the possibility of phase detection on fully embedded nanoparticles.

[1] García, Ricardo; Pérez, Rubén. Surf. Sci. Rep. 47, 197 (2002)

[2] M. Hanif, R. Juluri, M. Chirumamilla, V. Popok. J. Polym. Sci. B 54, 1152 (2016)

O 49.20 Tue 18:15 Poster A

Low-temperature STM measurements on the stable phase of Ge$_1$Sb$_2$Te$_4$ grown by MOVPE — •Philipp Küppers[1], Christian Holl[1], Marcus Liebmann[1], Albert Ratajczak[2], Detlev Grützmacher[2], Hilde Hardtdegen[2,3], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen — [2]Peter-Grünberg-Institut 9, Forschungszentrum Jülich — [3]Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen 2, Forschungszentrum Jülich

Ge$_1$Sb$_2$Te$_4$ is a phase change material, similarly used in DVDs and random access memory. It exhibits a metastable and a stable crystalline phase which differ only by their stacking sequence. Here, we study the stable phase of Ge$_1$Sb$_2$Te$_4$, grown by metalorganic vapor phase epitaxy (MOVPE) using scanning tunneling microscopy (STM) and spectroscopy at 6 K. We present atomically resolved flat and defect-free terraces as large as $30 \times 30\,\mathrm{nm}^2$ revealing a Te termination. Local density of states (LDOS) measurements show subsurface defects as triangular features in LDOS maps. While contacting the sample with a Cr (W) tip such that the resistivity decreases to $\approx 10^4\,\Omega$, we observe an additional sharp drop in resistivity by an order of magnitude after ramping the voltage to 0.8 V (1.1 V). The process is reversible by removing and recontacting the tip at the same position. Possible explanations of the switching process are discussed.

O 49.21 Tue 18:15 Poster A

Controlling telegraph noise in a few donor system by laser illumination — •Ole Bunjes, Philipp Kloth, Judith von der Haar, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Extending a low-temperature Scanning Tunneling Microscope with optical excitation, we have investigated the effect of laser-induced minority charge carriers on temporal charge fluctuations within the tip-induced space charge region (SCR) on the (110) surface of n-doped GaAs. Discrete charging events in GaAs cause the tunneling current to switch abruptly between well-defined values [1], a signature referred to as telegraph signal. We investigated the temporal characteristic of the underlying single-electron charging events with a spatial resolution on the atomic scale by recording a time series of the tunneling current at every tip position. We studied the variation of the telegraph signal in the presence of laser-induced free charge carriers in the SCR. Reduction of the current*s noise originating in the telegraph signal is found for small but non-vanishing hole concentrations, using the tunneling current as control parameter [2]. We attribute the reduction of the telegraphic step height to the photo-generated low-density hole gas that homogenizes the potential landscape at the sample surface. We acknowledge the financial support by the SFB1073 C04. [1] K. Teichmann et al., Nano Lett. 11, 3538-3542 (2011) [2] P. Kloth et al., Nat. Commun. 7, 10108 (2016)

O 49.22 Tue 18:15 Poster A

Nanosecond laser-induced periodic surface structures on fused silica dependent on additional confinement layer stacks — Martin Ehrhardt[1,2], •Pierre Lorenz[2], Shengying Lai[2], Frank Frost[2], Bing Han[1], and Klaus Zimmer[2] — [1]Advanced Launching Co-innovation Center, Nanjing University of Science and Technology, 200 XiaoLingWei, 210094 Nanjing, Jiangsu, China —

^{2}Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, 04318 Leipzig, Germany

Laser-induced periodic surface structures (LIPSS) are generated in semiconductor, polymer, metal and dielectric surfaces irradiated with short and ultra-short laser pulses. LIPSS generation with nanosecond laser pulses shows a dependency of the periodicity and the ripple orientation on the wavelength as well as the polarization of the laser beam. In the present study, LIPSS formation on fused silica surfaces covered by a layer stack system was studied. The layer stack system consist, start from the fused silica surface, of a polymer or semiconductor interface layer, a metal absorber layer and a photoresist confinement layer. The resultant LIPPS structures were analyzed by atomic force (AFM) and scanning electron microscopy (SEM). It was found that the LIPSS periodicity and height is dependent on the thickness and the material properties of the layers.

O 49.23 Tue 18:15 Poster A

Charge distribution within nanostructures of molecular dipoles on Au(111) — •Sergey Trishin^1, Daniela Rolf^1, Philipp Rietsch^2, Christian Lotze^1, Siegfried Eigler^2, and Katharina J. Franke^1 — ^{1}Freie Universität Berlin, Fachbereich Physik — ^{2}Freie Universität Berlin, Institut für Chemie und Biochemie

Donor-acceptor molecules have been investigated widely, because they offer suitable electronic characteristics for a possible use in electronic devices, such as single-molecule diodes or transistors. When deposited on a surface, the charge distribution within the molecule may change significantly due to screening and hybridization effects. Here, we investigate the N_2-ethane-tetracyano-quino-dimethane molecule on a Au(111) surface, which exhibits a large dipole moment in gas phase. On the Au(111) substrate, the molecules form ordered self-assembled chains of varying width. Employing non-contact AFM at low temperature, we measure the local contact potential difference (LCPD). We show that the molecules still exhibit a distinct dipole character on the substrate. The dipole moment depends on the width of the molecular chains.

O 49.24 Tue 18:15 Poster A

Ion beam induced surface patterns - All coefficients for the equation of motion from Monte Carlo simulations — •Hans Hofsäss, Omar Bobes, and Alrik Stegmaier — II. Physikalisches Institut, Universität Göttingen, Germany

Linear theories of surface pattern formation typically consider curvature dependent effects related to the 1^{st} order moments of the erosion, redistribution and implantation crater functions. Smoothing of a surface is described by either thermal surface diffusion or ion-induced viscous flow. The equation of motion (EOM) of the surface h(x,y,t) then consists of 1^{st} and 2^{nd} order spatial derivatives and a 4^{th} order term related to smoothing. Using the Monte Carlo simulation codes SDTrimSP we calculate all crater function moments (erosion, redistribution and implantation) up to 4^{th} order and derive all coefficients for the EOM up to 4^{th} order, including the non-linear coefficients. The calculation is applicable to almost any ion-target combination up to ion energies of several 10 keV, any ion incidence angle, and may include dynamic changes of the target stoichiometry. Higher order crater function moments give rise to a wavelength dispersion of the ripple propagation velocity and contributions similar to a diffusion term. Nonlinear coefficients related to derivatives $(dh/dx)^2$,$(dh/dx)^3$,$(dh/dy)^3$, $(dh/dx)(dh/dx)^2$ give rise to amplitude saturation and terrace formation. We calculate the complete set of coefficients using SDTrimSP for several model cases, which are then used as input for a software package that allows the simulation of dynamics for arbitrary, nonlinear EOMs.

O 49.25 Tue 18:15 Poster A

Transport-based single-atom STM electron-spin resonance: a cotunneling description — •Jose Reina^1, Nicolas Lorente^1, and Fernando Delgado^2 — ^{1}Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, Manuel de Lardizabal 5, E-20018 San Sebastián, Spain. — ^{2}Departamento de Física, Universidad de La Laguna, Instituto de estudios avanzados (IUdEA), Avda. Astrofísico Francisco Sánchez, S/N 38203 La Laguna (Tenerife), Spain

Electron spin resonance (ESR) has recently overcome its main limitation, reaching the single atom detection limit[1]. In its new form, magnetic resonance is observed as a variation of the current flowing through a scanning tunneling microscope tip positioned over a magnetic adatom while applying an ac. voltage of different frequencies. Although several theoretical origins of the ESR signal have been proposed [2], it is still unclear how the time-varying bias voltage couples to the localized spin, with marked discrepancies with the experimental observations. Here we show that this signal is associated to the variation of the potential energy felt by the electrons on its occupation of the adatom energy levels. Thus, by using a time-dependent cotunneling description of the transport, we estimate the STM-ERS driving strength and its dependence with the main control parameters of the ERS setup, making a close comparison with the experimental findings.

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

[2] P. Berggren and J. Fransson, Sci. Rep. 6, 25584 (2016). J.L. Lado, A. Ferrón, and J. Fernández-Rossier, Phys. Rev. B 96, 205420 (2017)

O 49.26 Tue 18:15 Poster A

Controlled soft-landing electrospray ion-beam deposition on freestanding graphene for high resolution transmission electron microscope characterization of molecules — •Suman Sen, Nilesh Vats, Stephan Rauschenbach, Sabine Abb, Wilfried Sigle, Marko Burghard, Peter van Aken, and Klaus Kern — Max Planck Institute for Solid State Research, Heisenbergstr.1, 70569 Stuttgart Germany

Electrospray ion-beam deposition (ES-IBD) has evolved as a pivotal technique for studying molecules in ultra-high vacuum (UHV) condition to attain single molecular resolution [1]. In this work, we deposited and learned about absorption properties of phosphotungstic acid (PTA) on single-layer graphene (SLG). We have demonstrated how large poly-oxo-metallate (POM) anions can be deposited in a controlled way with different landing energies on SLG in UHV. We showed that, PTA molecules have higher affinity to absorb onto amorphous impurity present on graphene compared to pristine SLG. Furthermore, atomic scale resolution of the PTA molecule absorbed on SLG using low-voltage (80 kV) aberration-corrected, high-resolution TEM was performed. Our study provides first detailed learning about the soft landing, absorption and characterization of individual POM anions on SLG. This can give insight into fabrication of two-dimensional materials involving graphene and POM species. [1] Rauschenbach, S. et al., Small, 2, 540-547, (2006)

O 49.27 Tue 18:15 Poster A

Self-assembly and charging of molecules on insulating films — Philipp Scheuerer and •Jascha Repp — University of Regensburg, Regensburg, Germany

Thick insulating films and bulk insulators enable the charging of adsorbates and have been used in studies to investigate charge transfer between individual molecules[1] and multiple charging of ensembles of molecules[2]. Self assembly on insulating films[3] allows one to investigate charging phenomena in ordered structures.

Here, we study self-assembled Perylenetetracarboxylic dianhydride (PTCDA) islands on a few layers of NaCl on Au(110). From AFM imaging with submolecular contrast, as well as dI/dV- and KPFS-measurements, we conclude that individual molecules in self assembled PTCDA islands can be charged. Furthermore, charges can be controllably transferred to neighboring molecules within a PTCDA island.

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

[2] P. Rahe et al., Nano Letters 16, 911 (2016)

[3] S. Burke et al., Nature Communications 6, 8312 (2015)

O 49.28 Tue 18:15 Poster A

Field emission investigations on flat polycrystalline Cu and Nb samples after argon-ion bombardment and pulsed laser treatment — •Süleyman Soykarci, Hendrik Bürger, Vitali Porshyn, Pavel Serbun, Dirk Lützenkirchen-Hecht, and Günther Müller — Bergische Universität Wuppertal, Gaußstr. 20, 42119 Wuppertal

In the present work, systematic investigations of polycrystalline Cu and Nb surfaces before and after Ar+ irradiation at 5 keV as well as laser treatments at different energies (300 uJ-2000 uJ) with a varying number of pulses (20-200) were performed by means of optical profilometry, atomic force microscopy and high-resolution scanning electron microscopy. In addition, local FE measurements were performed using a tungsten truncated cone needle anode in a field emission scanning microscope [1]. The results of ion bombardment indicated that the first detectable changes of the Cu and Nb surfaces occurred already after 3 min of ion bombardment. A reduction of the β-factors of sharp emitters was observed, resulting in an increase of the onset field values. The measurements on laser treated Nb samples showed an increase of the initial surface roughness values, however local field emission measurements (Øa= 30 um, z = 11 um) showed that the onset field for FE shifted to E > 700 MV/m. Detailed results will be presented and discussed at the conference. The work is funded by BMBF project 05H2015. [1] D. Lysenkov and G. Müller, Int. J. Nanotechnology 2, 239 (2005).

O 49.29 Tue 18:15 Poster A

Ultrahigh vacuum piezo-based mask aligner for shadow mask evaporation with sub-100 nm precision — •Priyamvada Bhaskar, Simon Mathioudakis, Tim Olschewski, Florian Muckel, Jan Rafael Bindel, Marcus Liebmann, and Markus Morgenstern — II. Institute of Physics B, RWTH Aachen University, 52056 Aachen, Germany

Realizing nanostructures in ultrahigh vacuum (UHV) could be beneficial for many experiments including the STM investigation of lateral interfaces or quantum transport experiments employing a 4-tip STM. Another example is to realize a clean interface for the detection of Majorana fermions, where in-situ evaporation of superconductors with pierced holes onto a topological insulator ($(\mathrm{Bi}_{x-1}\mathrm{Sb}_x)_2\mathrm{Te}_3$) is a controllable setup. Using three piezo-drivers on the mask aligner and three capacitive sensors on the shadow mask, the sample-mask distance can be controlled with a sub-100 nm precision and the mask can be aligned parallel to the sample surface. Mask and sample can be exchanged in-situ and the sample can be moved laterally with respect to mask using an additional piezo motor. The precise control of the mask-sample distance allows to minimize the penumbra of evaporated regions and improves the quality of the lateral interface. We demonstrate μm-sized patterns of Au on Si(100) with penumbra as low as 90 nm and show that the penumbra increases with increasing mask-sample distance.

O 50: Poster: Nanostructures on Surfaces II

Time: Tuesday 18:15–20:30 Location: Poster B

O 50.1 Tue 18:15 Poster B

Vibrational properties of the Au-($\sqrt{3} \times \sqrt{3}$)/Si(111) surface reconstruction — •S. Sanna[1], M. Krenz[2], S. Neufeld[2], W. G. Schmidt[2], E. Speiser[3], J. Räthel[3], S. Chandola[3], N. Esser[3], B. Halbig[4], M. Liebhaber[4], U. Bass[4], and J. Geurts[4] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen — [2]Department Physik, Universität Paderborn — [3]Leibniz-Institut für Analytische Wissenschaften, Berlin — [4]Physikalisches Institut, Experimental Physics 3, Universität Würzburg

The atomic structure of the Au-induced $\sqrt{3} \times \sqrt{3}$ reconstruction of the Si(111) surface has been controversially discussed for two decades. Different structural models have been proposed to explain the observed STM Pattern [J. Phys. Condens. Matter **27**, 475001 (2015)]. While the proposed structural models are almost energetically degenerate, the analysis of the vibrational properties might help to assign a structural model to the surface reconstruction. Our first principles calculations within density functional theory predict surface localized phonon modes for all investigated structures. However, the calculated Raman spectra are model-dependent. Corresponding surface Raman measurements reveal the presence of vibrational eigenmodes in the spectral range from 20 to 450 cm^{-1}, which are compatible with the frequencies calculated for the conjugate honeycomb-chained-trimer model (CHCT) [Surf. Sci. 275, **L691** (1992)]. On the basis of the phonon eigenfrequencies, symmetries, and Raman intensities, we assign the measured spectral features to the calculated phonon modes.

O 50.2 Tue 18:15 Poster B

Density functional theory investigation of rare earth silicide nanowires — •Kris Holtgrewe[1], Wolf Gero Schmidt[2], and Simone Sanna[1] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Department Physik, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn

Quasi one-dimensional electron systems are of fundamental interest both because of their unusual physical properties and for devices on nanometer scale. A prototype for these systems are rare earth (RE) silicide nanowires on silicon(001) surfaces. They grow self-organized controlled by macroscopic parameters such as temperature and amount of deposited RE.

Unfortunately, the knowledge about nanowires' detailed atomic structure, which is crucial for understanding their physical properties, is still incomplete. We have investigated different wire models from first-principles within density functional theory (DFT). Thereby erbium is chosen as a prototypical trivalent rare earth ion, its 4f-electrons treated as frozen states in the atomic core.

We categorized the models corresponding to six degrees of freedom: width, height, depth of burial, unit cell orientation, roof reconstruction and the underlying bulk RE silicide structure (hexagonal/tetragonal). After comparing the formation energy within ab-initio thermodynamics, electronic band structures and densities of states are calculated for the stable wires. Structural and electronic properties are discussed and compared with available STM, STS and ARPES measurements.

O 50.3 Tue 18:15 Poster B

Atomic-scale Au chains on Si(553): Influence of Defects — •Christian Braun and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Germany

One-dimensional atomic-scale metallic nanowires are popular model systems to study phenomena of one-dimensional physics such as Peierls instabilities, spin-charge separation, and charge-density waves [1]. Defects may be used to tune the nanowire properties, e.g., the electron transport or phase transition temperature. Recently it was shown that additional Si adatoms on Si(775)-Au induce local spin-polarization at the step [2]. In the present work the influence of Si adatoms and small molecules on the atomic structure and electronic properties of Si(553)-Au is investigated. For that purpose, density functional theory calculations are combined with ab initio thermodynamics. We discuss the defect impact on the Au chain dimerization, electronic band structure and predict desorption temperatures for foreign adsorbates.

[1] T Frigge, B Hafke, T Witte, B Krenzer, C Streubühr, A Samad Syed, V Miksic Trontl, I Avigo, P Zhou, M Ligges, D von der Linde, U Bovensiepen, M Horn-von Hoegen, S Wippermann, A Lücke, S Sanna, U Gerstmann, WG Schmidt, Nature 544, 207 (2017)
[2] J Aulbach, SC Erwin, R Claessen, J Schäfer, Nano Letters 16, 2698-2704 (2016)

O 50.4 Tue 18:15 Poster B

Spectral signatures of spin-charge separation in MoS_2 mirror twin boundaries — •Philipp Weiss[1], Wouter Jolie[2,3], Clifford Murray[2], Joshua Hall[2], Arkady Krasheninnikov[4], Hannu-Pekka Komsa[5], Carsten Busse[2,3,6], Thomas Michely[2], and Achim Rosch[1] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]Institute of Physics II, University of Cologne, Germany — [3]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [5]Department of Applied Physics, Aalto University, Finland — [6]Department Physik, Universität Siegen, Germany

We calculate the local spectral density of a one-dimensional metallic wire of finite length as predicted by Luttinger liquid theory. Fourier transformation in space yields the linear dispersion of spin and charge density waves which are the fundamental excitations of the system.

We apply this theory to recent STM measurements in MoS_2 mirror twin boundaries. Due to the metallic nature of these one-dimensional structures one can expect to find signatures of spin-charge separation in the STM signal. By means of the Fourier analysis we are able to extract spin and charge velocities from the experimental data. This indicates that a Luttinger liquid is likely realized in such grain boundaries.

O 50.5 Tue 18:15 Poster B

Gold-induced Surfaces on Stepped Germanium: Towards Atomic Models — •Tim Wagner, Julian Aulbach, Ralph Claessen, and Jörg Schäfer — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg

Self-assembly of gold atoms on terraced Si(hhk) or Ge(hhk) substrates stabilizes certain surface orientations. While Si(553)-Au and Si(557)-

Au have already been thoroughly examined, showing honeycomb step edges with regular arrays of spins, the atomic structure of the related Ge(hhk)-Au systems has not yet been determined. In order to investigate the influence of the substrate on the atomic structure, we perform scanning tunneling microscopy and low energy electron diffraction measurements on Ge(hhk)-Au surfaces. Based on our results, we propose first atomic structure models for Ge(221)-Au, Ge(335)-Au and Ge(557)-Au taking into account the known structural motifs of the Si(hhk)-Au family [1] and of the metal-induced Ge(111)-M systems [2]. While the Ge(335)-Au and Ge(557)-Au surface reconstructions display a great resemblance to their Si(hhk)-Au counterparts, in the special case of Ge(221)-Au the missing registry shift between neighboring step edges imposes an unusual rectangular unit cell, giving rise to a potentially different kind of inter-step correlation.

[1] J. Aulbach et al., Nano Lett. 16(2698) (2016).

[2] A. Tomaszewska et al., Ultramicroscopy 111(392) (2011).

O 50.6 Tue 18:15 Poster B

Temperature-dependent order-disorder transition in the Si(553)-Au nanowire system — •Bernd Hafke, Tim Frigge, Tobias Witte, Boris Krenzer, and Michael Horn-von Hoegen — Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg

Deposition of 0.5 ML Au on Si(553) at 650 °C results in the formation of Au double-strand chains with a twofold periodicity along the terraces of the vicinal Si surface. These metallic wires are structurally terminated by Si step edge atoms, where every third atom exibits a dangling bond leading to a threefold periodicity. Theory predicts magnetic properties of these interacting half-filled Si step edge atoms [1,2]. The long-range interaction of the twofold and threefold periodicity is investigated by spot-profile analysis in LEED at sample temperatures between 60 K and 180 K. The correlation length of Si step edge atoms along and perpendicular to the steps abruptly decreases upon heating above a temperature of $T \approx 100$ K, respectively. Interestingly, the streak-like intensity, indicative for the twofold periodicity of the Au atoms, shows an opposite behavior, i.e., an increase in correlation lenth upon heating. These findings are explained within a scenario of an order-disorder transition accompanied with the creation of so-called heavy and light zerodimensional domain boundaries.

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. **1**, 58 (2010).

[2] B. Hafke, *et al.* PRB **94**, 161403(R) (2016).

O 50.7 Tue 18:15 Poster B

Coupling of structural and electronic properties in 4/3-ML Pb/Si(111) investigated by femtosecond time- and angle-resolved 2PPE — •Abdul Samad Syed, Manuel Ligges, Vesna Mikšić Trontl, Peter Kratzer, and Uwe Bovensiepen — Fakultät für Physik, Universität Duisburg-Essen, Germany

Electronic properties and atomic structure of low dimensional systems determine each other. Scattering at steps was found, e.g., for Pb/Si(557) to lead to different electron relaxation for step down and step up directions [1]. A related, problem appears for threefold symmetry of Pb/Si(111)-($\sqrt{3} \times \sqrt{3}$) and we report here on the unoccupied electronic structure along $[\bar{1}\bar{1}2]$ and $[11\bar{2}]$ investigated by femtosecond time- and angle-resolved two photon photoemission (2PPE). Three electronic features dispersing along $k_x \parallel [\bar{1}\bar{1}2]$ were identified with binding energies 3.65, 3.5, and 3.3 eV above the Fermi level. In angle-resolved measurements the observed electronic states show for opposite momenta $k_x > 0$ and $k_x < 0$, an asymmetric intensity $I(k_x)$ and the electronic structure that appears to be different. In time-resolved experiment we find a momentum dependent change in the electron relaxation time $\tau(k_x)$. Polarization dependent studies reveal a different orbital character for the different states and for opposite k_x. We conclude to have identified the unidirectional anisotropy in the real and imaginary part of the electron self energy originating from the threefold surface symmetry of Pb/Si(111)-($\sqrt{3} \times \sqrt{3}$).

This work is funded by the DFG through research unit FOR 1700.

[1] A. Samad Syed et al., Phys. Rev. B **92**, 134301 (2015).

O 51: Poster: Electronic Structure of Surfaces: Spectroscopy, Surface States

Time: Tuesday 18:15–20:30 Location: Poster B

O 51.1 Tue 18:15 Poster B

Unoccupied electronic structure of the giant Rashba system Bi/Ag(111) probed by two-photon photoemission — •Philipp Rosenzweig[1,2], Sebastian Otto[1], and Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstr. 7, D-91058 Erlangen, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We probe the unoccupied band structure of the $(\sqrt{3} \times \sqrt{3})R30°$ substitutional surface alloy Bi/Ag(111)—from the Fermi to the vacuum level—by time- and angle-resolved, mono- and bichromatic, polarization-dependent two-photon photoemission (2PPE) at photon energies ranging from 1.51 to 4.89 eV. The obtained 2PPE patterns in $\overline{\Gamma \mathrm{M}}$ direction are exceptionally rich in structure, revealing pronounced contributions from the Rashba-split sp_z and p_xp_y ($m_j = 1/2$) initial states. The latter state is found to disperse downwards from (0.65 ± 0.03) eV above the Fermi level with a Rashba parameter of (3.0 ± 0.5) eVÅ—consistent with DFT calculations [1] and previous experiments [2, 3]; the corresponding lifetime is extracted as (26 ± 5) fs. The higher-lying, fully unoccupied p_xp_y ($m_j = 3/2$) surface state can also be identified in remarkable agreement with theory [1]. Close to the vacuum level, the 2PPE patterns reveal signatures of three image-potential resonances and the unoccupied Ag bulk *sp* band.

[1] Bihlmayer et al., Phys. Rev. B **75,** 195414 (2007).

[2] El-Kareh et al., Phys. Rev. Lett. **110,** 176803 (2013).

[3] Wissing et al., Phys. Rev. Lett. **113,** 116402 (2014).

O 51.2 Tue 18:15 Poster B

Electron-electron coincidences from surfaces - The new CoESCA station at Bessy II — •Torsten Leitner[1,2], Ieva Bidermane[1,3], Ruslan Ovsyannikov[1,3], Frank O. Schumann[4], Svante Svensson[1,2], Alexander Föhlisch[1,3], and Nils Martensson[1,2] — [1]UBjL - Uppsala-Berlin joint Laboratory, Berlin, Germany — [2]Uppsala University, Sweden — [3]Helmholtz-Zentrum Berlin, Germany — [4]Max-Planck Institut für Mikrostrukturphysik, Halle, Germany

We introduce the new CoESCA experimental station for electron-electron coincidences from surfaces, which is open for external users at the BESSY II synchrotron facility. The station is equipped with two Angular-resolved Time-Of-Flight (ArTOF) electron spectrometers and a state-of-the art sample manipulation and preparation system. We show first results from photo electron - Auger electron coincidences from Ag and present an outlook on future research opportunities.

O 51.3 Tue 18:15 Poster B

Electron-Rich surface of thin La$_{0.7}$Sr$_{0.3}$MnO$_3$ films revealed by Surface-Enhanced Raman Spectroscopy — •Sebastian Merten, Vitaly Bruchmann-Bamberg, Bernd Damaschke, Konrad Samwer, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Perovskite manganites are appealing materials for various potential applications in spintronics, catalysis or fuel cells. For all of them the electronic and atomic structure of the surface/interface is crucial for the performance of the future device. Unfortunately, the understanding of the manganite surface is still in its infancy. Surface-Enhanced Raman (SER) Spectroscopy represents a versatile tool to simultaneously probe different degrees of freedom and the small penetration depth of the surface plasmon (< 5nm) limits the probing area to the surface layers. Here, we present a detail SER study of thin La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) films grown on different substrates. SER spectra reveal a Jahn-Teller (JT) dominated surface structure, in contrast to the "bulk" Raman spectra where the JT modes are suppressed due to the rhombohedral structure of LSMO. Our experiments confirm theoretical calculations, which show a charge-transfer from the bulk to the surface and thus, formation of Mn^{3+}-ions at the surface. Furthermore, an enhancement of a specific JT mode depending on the epitaxial strain was observed. Temperature-dependent measurements reveal a second transition temperature at around $T = 260$ K. Financial support from DFG via SFB 1073 (TP B01, B04 and A02) is acknowledged.

O 51.4 Tue 18:15 Poster B

Potassium Doping of a Correlated Triangular Adatom Lattice — •Julian Maklar, Florian Adler, Jörg Schäfer, and Ralph Claessen — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg, Germany

Triangular lattices of localized electrons exhibit a rich phase diagram including spin liquids and exotic superconductivity due to geometric frustration and electronic correlations. Yet, the conditions for these regimes are not fully explored, as experimental realizations are rather limited. The focus of our research is on submonolayer triangular lattices of group IV adatoms on semiconductor substrates. Due to their simplicity and tunability by variation of adatoms and substrates, this material class can serve as a model system to study electronic correlations and frustration.

In this study utilizing ARPES and STM we investigate electron doping by K deposition on a triangular Sn atom lattice on Si(111). At low temperatures, Sn/Si represents a Mott-insulator with row-wise antiferromagnetic order, evident from backfolding of the Sn surface band. Upon K deposition, surprisingly a metal-insulator transition does not emerge. Instead we detect a sharpening of the Sn band followed by a rigid band shift towards higher binding energies. Furthermore, signatures of antiferromagnetic order are destroyed. STM measurements reveal a honeycomb reconstruction of K atoms on the Sn lattice after a deposition of 1/6 monolayer. This setup opens the door to search for exotic states of matter, specifically topological superconductivity.

O 51.5 Tue 18:15 Poster B

Scattering at single, non-magnetic bulk impurities in Cu — •Thomas Kotzott, Henning Prüser, and Martin Wenderoth — IV. Physikalisches Institut - Solids and Nanostructures, Georg-August-Universität Göttingen, Germany

The scanning tunneling microscope is most commonly used as tool for surface science. However, making use of the electron focusing effect the STM can also give an insight into the solid and then reveals a powerful combination of atomic lateral resolution and probing bulk properties. Here, we investigate the scattering process of bulk electrons at single, non-magnetic impurities and compare the properties of Ge with Ag within a Cu crystal.

Dilute alloys of Ge/Ag in Cu are prepared in-situ under UHV conditions. Cu and the impurity material Ge/Ag are simultaneously evaporated from electron beam evaporators onto a single crystal Cu(100) surface. STM and STS was performed using a home-built low-temperature setup operating at 6 K and $p < 5 \cdot 10^{-11}$ mbar.

Topography data reveals ring-like features in the local density of states with electronic contrasts down to few picometers in height. These signatures are attributed to the electrons being scattered at the impurity and propagating along the distinguished paths of electron focusing. Spectroscopy accesses the differential conductance with energy resolution and therefore resolves the scattering of different bulk states at the impurity. Comparing different non-magnetic impurities allows to expand the understanding of scattering processes on the atomic level.

O 51.6 Tue 18:15 Poster B

Numerical Calculations of Metastable Induced Electron Spectra (MIES) — •Tobias Bernd Gäbler, Wichard J. D. Beenken, and Erich Runge — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

We present ab initio calculations of the transition rates of the Auger de-excitation of metastable helium interacting with molecules. Following the simplifying assumptions by Kantorovich et al. [Surf. Sci. 444, 31 (2000)], we calculated the exchange matrix-elements relevant for the de-excitation by a MATLAB program based on molecular orbitals as result from standard quantum-chemical software packages like Gaussian. Thereby, density functional theory (B3LYP) and the Hartree-Fock method can be utilized. Both methods show only slight differences in the calculated transition rates. However, the Hartree-Fock method may be theoretically better justified for the applicability of the Koopman's theorem, and practically preferable due to a better correspondence of calculated ionization energies with the peak positions in measured MIES spectra. We will demonstrate calculated MIES spectra averaged over given trajectories of Helium atoms along the molecule.

O 51.7 Tue 18:15 Poster B

Probing low-energy correlations on μm length-scales with ultimate energy and momentum resolution — •Eike F. Schwier[1], Hideaki Iwasawa[2], Mashashi Arita[1], Hitoshi Takita[3], Umut Mansur[3], Akihiro Ino[1], Hirofumi Namatame[1], Masaki Taniguchi[1], Yoshihiro Aiura[4], and Kenya Shimada[1] — [1]Hiroshima Synchrotron Radiation Center, Hiroshima University, 2-313 Kagamiyama, Higashi-Hiroshima, Hiroshima 739-0046, Japan — [2]Diamond Light Source, Harwell Science and Innovation Campus, Didcot OX11 0DE, United Kingdom — [3]Graduate School of Science, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima 739-8526, Japan — [4]National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, Japan

We have developed a μ-ARPES system by combining the advantages of conventional high-resolution laser ARPES and spatially-resolved scanning PES. We use an optical lens system to focus our laser beam down to 5 μm and harness the available spatial resolution by using an XYZ stage with sub-μ precision of movement. Our μ-ARPES machine is able to revealed both intrinsic and extrinsic spatial inhomogeneity in the electronic structure with outstanding accuracy and more generally allows to choose surface regions and light conditions that greatly improve on conventional ARPES results. Here we present examples of our machines performance, focusing on spatially resolved measurements with high energy and/or angular resolution of superconducting materials and topological insulators.

O 51.8 Tue 18:15 Poster B

Quantifying the charge density wave properties in VSe$_2$ — •Timo Knispel[1], Wouter Jolie[1,2], Niels Ehlen[1], Konstantin Nikonov[1], Carsten Busse[2,3], Alexander Grüneis[1], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität — [3]Department Physik, Universität Siegen

We use scanning tunneling microscopy and spectroscopy (STS) to image the charge density wave (CDW) at the surface of VSe$_2$ and to probe its local density of states. Angle-resolved photoemission and tight-binding calculations are used to link the main features observed in STS spectra to contributions of the p-like and d-like bands of VSe$_2$. A transparent method to estimate the partial CDW gap based on STS spectra is provided. The estimated CDW gap of 26 ± 6 meV is is in good agreement with the transition temperature of VSe$_2$, pointing to weak electron-phonon coupling. This leads to the conclusion that the Peierls model of Fermi surface nesting is applicable in this material. The role of defects is investigated, which reveals that the partial gap in the density of states and hence the CDW itself is extremely stable, though the periodic modulation and amplitude of the CDW on the surface are strongly perturbed.

O 51.9 Tue 18:15 Poster B

The 2x1 reconstruction of the LaB6 (001)-surface observed by Scanning Tunneling Microscopy — •Philipp Buchsteiner[1], Jan Voigt[1], Geetha Balakrishnan[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Department of Physics, University of Warwick, United Kingdom

Lanthanum Hexaboride (LaB6) is widely used as cathode emitter due to its chemical stability and low work function of the (001)-surface [1]. We investigate the (001)-surface obtained by in situ cleavage at room temperature. The sample is directly transferred to our home built low temperature (6 K) Scanning Tunneling Microscope (STM). Our measurements unravel for the first time that a chain-like 2x1 reconstruction is present at the surface. Since LaB6 is built from positively charged La ions and negatively charged B6 molecules such an arrangement can avoid an unfavourable surface polarization. Such a 2x1 reconstruction has been observed for cleaved Samarium Hexaboride (SmB6) (001)-surfaces as well [2]. However, this modification has not been found on heated LaB6 (001)-surfaces, where only non-reconstructed areas with numerous vacancies have been observed [3]. Contrarily to this findings non-reconstructed areas obtained by cleavage do not exhibit such a high vacancy concentration. This work is supported by the DFG. [1] M. Trenary, Sci. Technol. Adv. Mater., 13 (2012) [2] S. Rößler et al., Philos. Mag., 96:31, 3262-3273 (2016) [3] J.S. Ozcomert, M. Trenary, Surf. Sci., 265 (1992)

O 51.10 Tue 18:15 Poster B

STM-Investigations of κ-(BEDT-TTF)$_2$X-Charge Transfer Salts — •Johannes Regel[1], Torge Mashoff[1], Harald Schubert[2], Michael Lang[2], Jens Müller[2], and Hans-Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz — [2]Physikalisches Institut, Goethe-Universität, Frankfurt

Organic charge-transfer salts of the κ-$(BEDT\text{-}TTF)_2X$ (short: κ-X) family share essential features with cuprates regarding their superconducting state. In both classes of materials, the electronic structure is quasi two dimensional and superconductivity emerges in the vicinity of the Mott insulating phase, resulting in a strong deviation of the superconducting properties from BCS theory.
We investigate small crystals of the two charge-transfer salts κ-$Cu[N(CN)_2]Br$ and κ-$Cu(NCS)_2$ using a low temperature scanning tunneling microscope and obtain good topographic resolution of the crystallographic structure. Due to the higher chemical pressure of κ-$Cu(NCS)_2$, the two salts differ in the proximity to the Mott phase. We use scanning tunneling spectroscopy to investigate this influence and the electronic properties of the samples.

O 51.11 Tue 18:15 Poster B

Growth studies and angle-resolved photoemission of Fe coatings on the topological Dirac semi-metal α-Sn — •Johannes Jehn, Victor Rogalev, Lenart Dudy, Jörg Schäfer, and Ralph Claessen — Physikalisches Institut und Röntgen Center for Complex Material Systems, Universität Würzburg, 97074 Würzburg, Germany

Topological materials like α-Sn exhibit a band inversion between the p-like conduction and s-like second valence bands. Being compressively strained in (001)-plane, α-Sn enters the Dirac semi-metal phase, with topological surface states (TSS) protected by time-reversal symmetry. A magnetic field breaks this symmetry and is expected to open a gap in the surface states.

We investigate the effect of Fe coatings deposited on α-Sn films grown *in situ* by MBE on InSb(001) substrates. In ARPES, α-Sn samples clearly show linear dispersing surface states with a Dirac point (DP) close to the Fermi level. The position of the DP is controlled by Te doping. Fe impurities are deposited flux-controlled on the surface of α-Sn films with a coverage ranging from sub-monolayer to several monolayers (determined from XPS). Theoretically, a ferromagnetic order mediated by the TSS might be conceivable in such samples. However, in ARPES we observe no gap opening at the DP within our resolution for all Fe coverages. We speculate that the presence of projected bulk states near the Fermi level disturbs the ferromagnetic coupling via the TSS.

O 51.12 Tue 18:15 Poster B

Electronic states on metal/topological insulator heterostructure — •Garima Saraswat, Jan Homberg, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Topological insulators (TI) are of great interest due to their unusual surface states. Exotic properties such as p-wave-like superconductivity and gapped Dirac states have been predicted for proximity coupled superconductor/TI and ferromagnet/TI structures respectively [1]. Normal metal/TI junctions which could be very relevant for device fabrication remain relatively unexplored. In this work we perform scanning tunneling spectroscopy (STS) on few monolayers of Pb deposited on Sb_2Te_3 single crystal surface. We observe a change in the Fermi level as a function of Pb coverage on the surface. Pb nanoislands exhibit quantum well states. The effect of topological surface states on these QW states will be discussed.

[1] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010)

O 51.13 Tue 18:15 Poster B

Symmetry in photoelectron angular distribution of black phosphorus — •Katharina T. Ritter[1], Kenta Kuroda[2], Takeshi Kondo[2], Takao Sasagawa[3], Koichiro Yaji[2], Shik Shin[2], and Markus Donath[1] — [1]Physikalisches Institut, University of Münster, Germany — [2]ISSP, University of Tokyo, Japan — [3]LMS, Tokyo Institute of Technology, Japan

Angle-resolved photoelectron spectroscopy (ARPES) is the technique to investigate the electronic structure of solids and molecules by measuring the photoemitted electron intensity versus their angular distribution or kinetic energy. Recently, the combination of ARPES with ab-initio electronic-structure calculations shows that the photoelectron angular distribution (PAD) can greatly give insights into electronic and structural properties of organic molecular layers [1]. However, the understanding of the PAD as a result of excitations from Bloch states in solids still remains challenging.

In this contribution, we apply this technique to electronic structure of black phosphorus (BP), which consists of puckered atomic layers coupled by weak inter-layer van der Waals forces. By using high-resolution ARPES combined with 7 eV laser light, we directly map the PAD. Remarkably, it is found that the PAD pattern sensitively depends on the linear polarization of the incident light. From this result, we discuss how the light polarization is related to the symmetry of the electronic state to give rise to the observed PAD pattern.

[1] J. Ziroff *et al.*, Phys. Rev. Lett. **104** (2010) 233004

O 51.14 Tue 18:15 Poster B

STM/AFM study of local work function variations on h-BN/Cu(111) — •Abhishek Grewal[1], Matthias Muenks[1], Yuqi Wang[1], Markus Ternes[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The adsorption of single atoms or molecules on surfaces is mediated by their interaction with the substrate. The surfaces must, therefore, be characterized and understood from the structural, chemical and electronic point of view. In this respect, the nanometer scale local work function variations of the hexagonal boron nitride (h-BN) decoupling layer have been used for explaining favorable adsorption sites and molecular arrangements [1,2]. Using a tuning-fork based combined STM/AFM at 1 K base temperature we study h-BN on a Cu(111) substrate. We find bias dependent electronic corrugations by analyzing constant current and constant height STM images. We compare the local work function variation obtained by field emission resonance states [3] and complimentary Kelvin probe force microscopy at the different areas of this corrugation. Analyzing three-dimensional force maps we do not observe the soft stiffness previously found on h-BN/Rh(111) samples [4].

1. H. Dil et al., Science 319, 1824 (2008).
2. P. Jacobson et al., Nat. Comm. 6, 8536 (2015).
3. S. Joshi et al., Nano Lett. 12, 5821 (2012).
4. T. Herden et al., Nano Lett. 14, 3623 (2014).

O 51.15 Tue 18:15 Poster B

Pb single atom contacts in a STM — •Jan Homberg, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

In scanning tunneling spectroscopy, superconducting tips may be used to achieve high energy resolution not limited by Fermi broadening. Here we use Pb tips on a Pb(100) single crystal to investigate single atom contacts. Multiple Andreev Reflections as well as Josephson supercurrents are observed and analysed giving insight into the electronic properties of the contacts.

O 51.16 Tue 18:15 Poster B

Investigation of Honeycomb-Iridate Surfaces by Means of STM and STS — •Thomas Dziuba[1], Felix Lüpke[1], Friedrich Freund[2], Soham Manni[2], Philipp Gegenwart[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Experimentalphysik VI, Universität Augsburg, Germany

Honeycomb iridates A_2IrO_3 ($A = Na$ or Li) have attracted much interest as prototype spin-orbit Mott insulators with magnetic Kitaev exchange interaction. They are also considered as promising candidates for novel correlated topological insulator behavior. This motivates detailed microscopic investigations of the surface properties by scanning tunneling microscopy (STM) and spectroscopy (STS). Honeycomb iridates consist of an alternating stacking of negatively charged honeycomb iridate structures and positively charged hexagonal alkali metal layers [1]. Optical conductivity indicates a large bulk bandgap ($340\,meV$ [2]). We found, that the surface of both, pure and partly Li-doped sodium iridate shows 1×1- and 3×1 reconstructions, that in all cases exhibit a surface band gap. This gap depends crucially on the particular reconstruction as well as on the alkali metal configuration, with higher Li-content leading to smaller bandgaps [1]. Recently, α-Li_2IrO_3 single crystals were synthesized [3]. We report first STM/STS measurements on them, revealing interesting surface properties. Work supported by DFG SPP1666. [1] F. Lüpke et al, Phys. Rev. B 91, 041405(R) (2015) [2] V. Hermann et al, Phys. Rev. B 96, 195137 (2017) [3] F. Freund et al, Sci. Rep. 6, 35362 (2016)

O 51.17 Tue 18:15 Poster B

Development of a multichannel spin detector for photoelectron spectroscopy with hard x-rays — •Matthias Schmitt[1], Alexander Wiegand[1], Lenart Dudy[1], Michael Sing[1], Ralph

Claessen[1], Sergey Chernov[2], Gerd Schönhense[2], Andrei Gloskovskii[3], Katrin Ederer[3], Christoph Schlueter[3], and Wolfgang Drube[3] — [1]Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems, 97074 Würzburg, Germany — [2]Universität Mainz, Institut für Physik, 55128 Mainz, Germany — [3]DESY Photon Science, 22607 Hamburg, Germany

Spin-resolved photoelectron spectroscopy is a powerful technique to directly probe the spin-polarized electronic structure of magnetic systems. However, conventional single channel spin detectors used for spin filtering and detection exhibit very low efficencies and, in addition, lack the possibility to benefit from the two-dimensional imaging capabilities of modern electron energy analyzers with respect to energy and angle. Thus, spin- and angle resolved measurements are in general cumbersome. This applies all the more for the hard x-ray regime where the photoabsorption cross sections are extremely small. Here we report on the development of a multichannel spin detector for hard x-ray photoelectron spectroscopy using a tungsten single crystal for spin-dependent low energy electron diffraction in 90° geometry. We also show first test measurements of magnetite with a spin polarization of -100% at the Fermi energy, performed at PETRA III in Hamburg, Germany.

O 51.18 Tue 18:15 Poster B

Comparative scanning tunneling spectroscopy study of cobalt oxide islands and thin films on Au(111) and Ir(100) — •Maximilian Ammon, Sara Baumann, Lutz Hammer, and M. Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Cobalt oxide is of great interest mainly due to its catalytic and magnetic properties [1-3]. It has been shown that cobalt oxide can be epitaxially grown on various single crystal surfaces of noble and transition metals [4-7].

Low-temperature scanning tunneling spectroscopy in ultra-high vacuum is used to study the electronic properties on a local scale. We compare cobalt oxide bi- and trilayer islands with a rocksalt structure on Au(111) [4,7] with corresponding cobalt oxide films on Ir(100). The measured local density of states (LDOS $\propto$ dI/dV) of the oxide is strongly reduced around E_F on both substrates, but the spectral shape varies significantly. On Au(111) the dI/dV signal is reduced to zero in an energy interval of up to 0.5 eV around E_F. In contrast on Ir(100) a sharp, symmetric dip is observed with finite dI/dV signal at E_F.

[1] Fester et al., Nat. Commun. **8**, 14169 (2017) [2] Liao et al., Nat. Nanotechnol. **9**, 69 (2014) [3] Skumryev et al., Nature **423**, 850 (2003) [4] Fester et al., Top. Catal. **60**, 503 (2017) [5] Heinz et al., J. Phys.: Condens. Matter **25**, 173001 (2013) [6] Schindler et al., Surf. Sci. **603**, 2658 (2009) [7] Chassé et al., Surf. Sci. **602**, 443 (2008)

O 51.19 Tue 18:15 Poster B

Probing magnetic interactions between transition metal atoms via YSR states — •Javier Zaldívar[1], Deung-Jang Choi[1,2,3], Carmen Rubio-Verdú[1], Miguel Moreno Ugeda[1], Jose Ignacio Pascual[1], Edwin Herrera[4], Isabel Guillamón[4], Hermann Suderow[4], Carlos García Fernández[3], and Nicolás Lorente[2,3] — [1]CIC nanoGUNE, San Sebastián, Spain — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), San Sebastián, Spain — [3]Donostia International Physics Center, San Sebastián, Spain — [4]Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center, UAM, Madrid, Spain

Recent studies proposed the formation of Shiba(YSR) bands in chains of magnetic atoms on superconductors in the presence of spin-orbit coupling as a platform to realize topological superconductivity[1]. However, construction of nanostructures on superconducting materials by atomic manipulation resulted elusive to date, preventing the study of the evolution from single-atom YSR states to Majorana chains.

We compare the YSR excitation spectra of nanostructures built with transition metal adatoms on the surface of β -Bi2Pd [2]. We show these excitations depend on the adsorption state, the mutual interaction, and also track variations due to magnetic fields. Our results provide an insight into the nature of magnetic interactions on a superconductor at the atomic scale at the early stages of chain formation.

[1] S. Nadj-Perge et al., Science 34, 6209 (2014)

[2] D. -J. Choi et al., arxiv: 1709.09224 (2017)

O 51.20 Tue 18:15 Poster B

Growth and electronic structure characterization of FeSe$_x$Te$_{1-x}$ thin films on a topological insulator — •Thiago R. F. Peixoto[1], Simon Müller[1], Sujit Manna[2], Jagadeesh Moodera[2], and Friedrich Reinert[1] — [1]Experimental Physics VII and Röntgen Center for Complex Materials, Universität Würzburg — [2]Department of Physics, Massachussets Institute of Technology, Boston, USA

The realization of a topological superconductor state at the interface between a strong three-dimensional topological insulator (3D-TI) and an s-wave superconductor is one of the central issues in condensed matter physics nowadays [1]. In iron-based superconductors, the presence of magnetic species may yet break the time-reversal symmetry of the TI non-trivial electronic structure, allowing the existence of chiral Majorana fermions [1]. Here we report the successful growth of high quality FeSe$_x$Te$_{1-x}$ films on 3D-TI (Bi,Sb)Se$_x$Te$_{3-x}$ substrates by means of molecular beam epitaxy. Low-energy electron diffraction (LEED) and X-ray photoemission spectroscopy (XPS) experiments confirm the formation of 1-2 unit cells Fe(Se,Te) film with a high surface quality. Angle-resolved photoemission spectroscopy (ARPES) has been performed at temperatures between 1 K and 20 K, at photon energies between 20 eV and 150 eV, and for both linear polarizations, showing typical signatures of the FeSeTe valence band structure along the surface high symmetry directions. Our data is discussed in comparison with well-established ARPES results and band structure calculations.

[1] L. Fu and C. L. Kane, *Phys. Rev. Lett.* **100**, 096407 (2008).

O 52: Poster: Electronic structure: Surface Magnetism and Spin Phenomena

Time: Tuesday 18:15–20:30 Location: Poster B

O 52.1 Tue 18:15 Poster B

Field and temperature dependent switching analysis of holmium single atom magnets — Fabian Donat Natterer[1], Fabio Donati[1,2,3], •Patrick Forrester[1], François Patthey[1], and Harald Brune[1] — [1]Institute of Physics, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland — [2]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Korea — [3]Department of Physics, Ewha Womans University, Seoul, Korea

As stable magnetic bits have shrunk to the fundamental limit of single atoms, questions about the thermal stability of magnetic information become pressing. Using the example of holmium single atom magnets on MgO, we investigate the magnetic bistability and switching between 4.3 K and up to 50 K. A coercive field of more than 8 T is found at 35 K. We encounter spontaneous magnetization reversal at about 45 K and 8 T in our STM study. We estimate the transverse magnetic anisotropy energy from a magnetic field and bias voltage dependent 2-state switching analysis at 4.3 K. This allows us to constrain the possible magnetic ground state to either $J_z = 8$ or $J_z = 7$, both explaining magnetic bistability at finite field strengths.

O 52.2 Tue 18:15 Poster B

Visualizing the magnetic structure of Fe bilayers on Ir(111) by atomic manipulation — Nadine Hauptmann[1], Melanie Dupé[2], •Tzu-Chao Hung[1], Alexander K. Lemmens[1], Jairo Sinova[3], Stefan Heinze[3], Daniel Wegner[1], Bertrand Dupé[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, Netherlands — [2]Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany — [3]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Chiral magnetic structures, in which Dzyaloshinskii-Moriya interaction plays an important role on the mechanism of stabilization, have been predicted being a candidate for spintronic applications. By utilizing the combination of spin-polarized scanning tunneling microscope (SP-STM) and magnetic exchange force microscopy (MExFM), or so-called SPEX, we get both the magnetic and geometric sensitivity down to the atomic scale. We apply this method to probe the magnetic structure of the bilayer of Fe on Ir(111), which reveals chiral magnetic order. However, both SP-STM and MExFM do not reveal magnetic contrast of the total unit cell, resulting from the strongly corrugated surface. Therefore, we use the manipulation of iron adatoms, which locally exchange couple with the underlying spin spiral, providing spin information in regions of the unit cell where no magnetic contrast can be observed in SPEX images of the bare surface.

O 52.3 Tue 18:15 Poster B

Scanning tunneling microscopy and spectroscopy of endohedral fullerenes on metallic substrates — •Emmanouil Koutsouflakis, Sebastian Schimmel, Zhixiang Sun, Denis Krylov, Danny Baumann, Alexey Popov, Bernd Büchner, and Christian Hess — Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany

Single Molecule Magnets (SMMs) are molecular materials whose molecules may exhibit magnetic properties such as magnetization under zero-field conditions, large relaxation times and high blocking temperatures. However towards molecular electronics and the subsequent controlled manipulation of single spins in SMMs, the obstacle of the insufficient chemical stability of many SMM architectures has to be overcome, in order to facilitate both their organization on substrates and the preservation of their properties.

We report on the investigation of resolving the limiting applicability of SMMs in molecular spintronics by the use of Endohedral Metallofullerenes (EMFs). We research on the alternative of the trimetallic nitride EMFs of the type $A_{3-n}B_nN@C_{80}$ (n=0-3; A, B rare earth metals or transition metals) where a carbon cage encapsulates a triangular cluster of three rare earth/ transition metal atoms and a nitrogen at its center. In particular, we evaporate Dy-based EMFs on metallic substrates and in order to probe the feasible monolayer coverage and to estimate the adsorption characteristics and the electronic structure of the deposited molecules we performed Scanning Tunneling Microscopy and Spectroscopy.

O 52.4 Tue 18:15 Poster B

Evolution of the Kondo effect in ConCum chains — •neda noei, alexander weismann, and richard berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, 24098 Kiel, Germany

Using a low temperature scanning tunneling microscope, monatomic Cu chains with lengths up to 100 nm were fabricated. By dipping the STM tip into Cu(111), different kinds of dislocations were generated. Among these dislocations, long Cu chains are an interesting system to investigate spin interaction between magnetic atoms. Two interacting magnetic atoms can be considered as a prototype system for spin exchange correlations. We attached Co adatoms to monatomic Cu chains to investigate how their adsorption sites and their distance from each other affect spin correlations between them. We observed a significant change of Kondo resonance when a Co atom was attached to the chain. This can be addressed to directional hybridization of Co atom d-orbitals to the chain. Moreover, by adding Co atom to the end of the chain, the Kondo resonance broadens appreciably. We have shown that the amplitude and width of Kondo resonance depends on the distance between Co atoms at chain.

O 52.5 Tue 18:15 Poster B

Yu-Shiba-Rusinov states of Fe adatoms on the quasi 2D superconductor $2H$-NbSe$_2$ — •Rojhat Baba[1], Eva Liebhaber[1], Sebastian Rohlf[2], Kai Rossnagel[2], Benjamin W. Heinrich[1], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany. — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany.

Magnetic impurities in superconducting materials induce Yu-Shiba-Rusinov (YSR) states inside the superconducting energy gap due to the exchange coupling between the impurity and the Cooper pair condensate. The superconductor $2H$-NbSe$_2$ is a transition metal dichalcogenide compound with a strong 2D character because of the weak van der Waals interaction between its layers. Furthermore, the material shows a transition to a charge density wave (CDW) state at low temperatures.

We use low temperature scanning tunneling microscopy and spectroscopy for the investigation of single Fe adatoms on $2H$-NbSe$_2$. The Fe adatoms reside in two different adsorption sites which induce significant differences in the energy of the d resonances as well as of the YSR states. A further characterization hints towards an influence of the CDW of the $2H$-NbSe$_2$ surface on the energy of the YSR states.

O 52.6 Tue 18:15 Poster B

Spin-resolved very-low-energy electron diffraction from ferromagnetic Fe films — •Christoph Angrick[1], Andre Reimann[1], Christian Thiede[1], Koji Miyamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]HiSOR, Hiroshima University, Japan

Spin-dependent electron scattering from ferromagnetic films is interesting for two reasons: (i) A ferromagnetic film can be used as a promising scattering target in spin-polarization analyzers as single [1,2] and multichannel devices [3,4]. Ferromagnetic films offer a high Sherman function and an easy way to reverse the asymmetry. (ii) Electron scattering experiments provide information about the surface barrier, which is predicted to be spin-dependent for ferromagnets [5].

We investigate ferromagnetic Fe films with spin-resolved very-low-energy electron diffraction by varying the electron kinetic energy and the incident polar as well as azimuthal angle over a wide range. In the focus of this work are two targets: (i) p(1x1)O-Fe(001)/MgO(001) and (ii) Fe(110)/W(110).

[1] Winkelmann *et al.*, Rev. Sci. Instrum. **79**, 083303 (2008)
[2] Okuda *et al.*, Rev. Sci. Instrum. **79**, 123117 (2008)
[3] Kolbe *et al.*, Phys. Rev. Lett. **107**, 207601 (2011)
[4] Tusche *et al.*, Appl. Phys. Lett. **99**, 032505 (2011)
[5] Burgbacher *et al.*, Phys. Rev. B **87**, 195411 (2013)

O 52.7 Tue 18:15 Poster B

Magnetic anisotropy of individual Fe and Co atoms on a MgO/Ag(001) substrate — •Stanislav Stupko[1], Eva Rauls[2], Wolf Gero Schmidt[1], and Uwe Gerstmann[1] — [1]University of Paderborn, Paderborn, Germany — [2]University of Stavanger, Stavanger, Norway

Combining high energy resolution of radio-frequency (RF) resonance methods with the spatial resolution and manipulation capabilities of scanning tunneling microscopy (STM) provide a promising avenue to study single-spin resonance at the nanoscale. Recent experiments study are promising by investigating single double-decker molecules(TbPc2) [1] and individual Fe- and Co-atoms placed on a magnesium oxide film [2]. In this work, we treat the system investigated in [2] with a full relativistic density-functional theory (DFT) approach (implemented in the Quantum ESPRESSO package), for all possible adsorption sites. Within non-collinear DFT, we compute the anisotropy of the magnetic properties, including the full EPR fingerprint. In particular, the orbital magnetization for the investigated periodic system is evaluated using a Berry-phase formula [3]. By this, we are able to clarify some open questions concerning Fe and Co adsorption, such as differences in STM/EPR signals for different Fe-atoms or their absence in case of Co-atoms.

[1] Müllegger et al., Phys.Rev.Lett. 113, 133001 (2014).
[2] Baumann et al., Science 350, 6259 (2015).
[3] Ceresoli et al., Phys.Rev. B 81, 060409(R) (2010).

O 53: Overview Talk: Olaf Magnussen

Time: Wednesday 9:30–10:15 Location: HE 101

Invited Talk O 53.1 Wed 9:30 HE 101

Elementary steps in surface dynamics and reactivity at electrochemical interfaces — •Olaf Magnussen — Institute of Experimental nad Applied Physics, Kiel University, Kiel, Germany

Processes at electrochemical interface are the key to many current and emerging technologies, e.g. in energy storage or micro- and nanofabrication. Detailed insights into these processes on the atomic scale can be obtained by fast in situ scanning tunneling microscopy (Video-STM) and novel synchrotron X-ray scattering techniques. These can provide data on the mechanisms and dynamics of adsorbate diffusion and interactions on the electrode surface and of structural changes during electrochemical reactions, as shown here for selected examples. First, the diffusion of isolated anionic, cationic, and organic adsorbates on noble metal electrodes will be discussed, indicating a decisive role of coadsorbed anionic species. Specifically, coadsorbates can induce an inverted potential dependence, suggesting that they can change the diffusion mechanism. Second, results on Pt oxidation and Pt oxide reduction are presented, which reveal fundamental differences between different surface orientations. While on Pt(111) oxygen ingress into the Pt surface is initially fully reversible, it results in irreversible structural changes on Pt(100).

O 54: Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures III

Organizers: Sabine Maier, FAU Erlangen-Nürnberg; Meike Stöhr, University of Groningen

(Synopsis provided with part I of this session)

Time: Wednesday 10:30–13:00 Location: MA 004

Invited Talk O 54.1 Wed 10:30 MA 004

Molecularly functionalized surfaces and interfaces — •Adam Foster — Department of Applied Physics, Aalto University, Finland — NanoLSI, Kanazawa University, Kanazawa 920-1192, Japan — Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128, Germany

Many ideas in next generation technology are predicated on atomic and molecular control of surfaces and interfaces. A natural route to providing this level of control is to design the interface directly using molecular building blocks via self-assembly. Using a combination of modelling approaches in partnership with Scanning Probe Microscopy experiments, in this work we consider several examples where the interface has been designed by the controlled assembly of molecular layers. We first introduce the computational tools at the heart of our methodology, and discuss the challenges when simulating complex assembly processes and comparing to experiment. We then compare the adsorption and reaction mechanisms on a benchmark insulator system [1], and also contrast to processes on conducting surfaces [2]. Finally, we build upon this to consider new insights offered by modern machine learning simulation approaches.

[1] J. Phys. Chem. C 120 (2016) 14730, Phys. Chem. Chem. Phys., 19 (2017) 15172

[2] J. Phys. Chem. C 120 (2016) 8772, Nat. Commun. 7 (2016) 11559, Nat. Commun. 7 (2016) 12711, ACS Nano 11 8122 (2017)

O 54.2 Wed 11:00 MA 004

Artificial Intelligence for Molecules on Surfaces — •Milica Todorović[1], Michael U. Gutmann[2], Jukka Corander[3,4], and Patrick Rinke[1] — [1]Aalto University, Espoo, Finland — [2]University of Edinburgh, Edinburgh, UK — [3]University of Oslo, Oslo, Norway — [4]University of Helsinki, Helsinki, Finland

Quantum mechanical accuracy is required to simulate the structures and properties of molecules on surfaces. However, accurate calculations are costly and extensive sampling is prohibitive, so studies into molecular assembly and surface-supported processes like diffusion are guided by human intuition. To promote unbiased studies into molecular surface structures and phenomena, we have combined atomistic simulations with Bayesian optimisation - an artificial intelligence (AI) technique designed for complicated optimisation tasks [1]. We demonstrate how the AI was adapted to learn surface and property landscapes of molecules on surface with minimal computational sampling [2], delivering most stable surface structures with favorable designer properties. Energy landscapes can be further data-mined for low energy paths and associated trajectories to reveal the atomistic mechanisms behind key processes. We showcase the capability of AI to infer complex properties on several examples of atomic and molecular surface adsorbates. [1] M.U. Gutmann and J. Corander, J. Mach. Learn. Res. 17, 1 (2016). [2] M. Todorović, M. U. Gutmann, J. Corander and P. Rinke, arXiv:1708.09274 (2017).

O 54.3 Wed 11:15 MA 004

Monte Carlo simulation of the 2D self-assembly of functional molecules — •Paweł Szabelski[1], Damian Nieckarz[1], and Wojciech Rzysko[2] — [1]Department of Theoretical Chemistry, Maria Curie-Skłodowska University, Lublin, Poland — [2]Department for the Modeling of Physico-Chemical Processes, Maria Curie-Skłodowska University, Lublin, Poland

Controlled self-assembly of molecular building blocks on solid substrates is a versatile method to create low-dimensional structures with preprogrammed morphology and functions. In this contribution, using theoretical tools, we demonstrate how the structure of large self-assembled molecular systems can be predicted based on individual properties of building blocks at play. In particular we focus on the role of directionality of interactions provided by discrete active centers being part of model star-shaped tectons. Our theoretical predictions are compared with available experimental data and hints on synthesis of organic functional molecules able to form various superstructures are given. The findings from the Monte Carlo modeling can be useful in designing of 2D supramolecular architectures as well as of covalently bonded structures resulting from on-surface polymerization reactions.

The financial support of the Polish National Science Centre (grant 2015/17/B/ST4/03616) is gratefully acknowledged

O 54.4 Wed 11:30 MA 004

Kinetic control in molecular self-assembly on an insulating surface — •Lev Kantorovich[1], Chiara Paris[1], Andrea Floris[1,2], Simon Aeschlimann[3], Julia Neff[3], Felix Kling[3], and Angelika Kühnle[3] — [1]King's College London, Strand, London, WC2R 2LS, U.K. — [2]University of Lincoln, Brayford Pool, Lincoln LN6 7TS, U.K. — [3]Johannes Gutenberg-University Mainz, Duesbergweg 10-14, 55099 Mainz, Germany

We present a new route for creating a set of metastable molecular architectures on surfaces. This approach relies on two key aspects: First, the suitable choice of the initial state of the molecules triggers a well-defined transformation path. Second, the observed path is entirely controlled by kinetics rather than thermodynamics. The feasibility of this route is demonstrated using a model system of dihydroxybenzoic acid molecules on the (10.4) surface of calcite. An initial state of molecular dimers undergoes, upon increase of temperature, a series of structural transitions from clusters to ordered striped and then dense networks, and finally to a disordered structure. Combining high-resolution dynamic atomic force microscopy experiments and density-functional theory calculations, we provide a comprehensive analysis of the fundamental principles driving this sequence of transitions. Our study opens new avenues based on kinetic control as a promising strategy for achieving tailored molecular architectures on surfaces.

O 54.5 Wed 11:45 MA 004

Bishop diffusion involving a chiral flip — •Simon Aeschlimann[1,4], Felix Kling[1], Chiara Paris[2], Andrea Floris[2,3], Lev Kantorovich[2], Ralf Bechstein[1], and Angelika Kühnle[1] — [1]Institute of Physical Chemistry, Johannes Gutenberg-University Mainz, Duesbergweg 10-14, 55099 Mainz, Germany — [2]Department of Physics, King's College London, London WC2R 2LS, United Kingdom — [3]School of Mathematics and Physics, University of Lincoln, Brayford Pool, Lincoln LN6 7TS, United Kingdom — [4]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany

Molecular surface diffusion is one of the most fundamental process in nature with far-reaching impact on a wide range of fields including, e.g., catalysis, sensing and surface functionalization. So far, molecular surface diffusion studies have mainly been limited to high-symmetry surfaces possessing rotational symmetry. Here, using the low-symmetry (10.4) surface of calcite, we present a novel molecular diffusion mechanism that can be described by the bishop move in chess, meaning that only half of the existing lattice sites are accessible for an individual molecular species. Interestingly, due to the only existing symmetry operation of the surface, a glide reflection symmetry, this bishop movement is inevitably associated with a flip in the chiral adsorption footprint of the molecular species towards the surface. Here, we demonstrate the pivotal influence of the surface symmetry on the detailed diffusion mechanism, including the adsorption chirality.

O 54.6 Wed 12:00 MA 004

Tuning the self-assembly of carboxyl-substituted triphenylamine-derivatives on bulk NaCl(001) and KBr(001) — •Mirunalini Devarajulu[1], Jia Liu[1], Min Ken Li[1], Christian Steiner[1], Bettina Gliemann[2], Yi Liu[1], Tuan Anh Pham[1], Milan Kivala[2], and Sabine Maier[1] — [1]Department of Physics, University of Erlangen-Nürnberg, Erlangen, Germany — [2]Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg, Erlangen, Germany

While most molecular self-assemblies so far have been studied on metallic substrates, comparatively little is known about molecular self-assemblies on insulating surfaces. One reason is the weak and often unspecific molecule-substrate interaction on bulk insulating surfaces. Therefore, the structure of the self-assemblies is challenging to predict. Here, we present a study on the self-assembly of a carboxyl-substituted dimethylmethylene-bridged triphenylamine derivative [1] on bulk NaCl(001) and KBr(001) by non-contact AFM at low temperature. The intermolecular hydrogen bonding contributes to the formation of 2D monolayers on NaCl(001) and KBr(001). We observed structurally different self-assemblies of the carboxyl-substituted triphenylamine derivative on NaCl(001) and KBr(001), respectively, due to a significant change in lattice mismatch [2]. The surface templating effect and binding motifs will be discussed in detail.

[1] C. Steiner et al. J. Phys. Chem. C, 2015, 119 (46), 25945-25955
[2] S. Maier et al. Phys. Rev. B, 2007, 75, 195408

O 54.7 Wed 12:15 MA 004

Porphyrins on Titania — •Thilo Glatzel[1], Res Jöhr[2], Antoine Hinaut[1], Silvio Decurtins[3], Shi-Xia Liu[3], Tobias Meier[1], Rémy Pawlak[1], and Ernst Meyer[1] — [1]University of Basel, Department of Physics, 4056 Basel, Switzerland — [2]Lehrstuhl für Angewandte Physik, Ludwig-Maximilians-Universität, 80799 Munich, Germany — [3]University of Bern, Department of Chemistry, 3012 Bern, Switzerland

Titania surfaces sensitized with metallo-porphyrins are of increasing interest for photocatalysis or photovoltaics. In these applications, the dye absorbs light and injects the exited electron into the conduction band of the titania. The binding configuration is thereby of great importance for the electron transfer process. To simultaneously investigate the binding configuration and its influence on the charge transfer process, nc-AFM and in particular KPFM are the methods of choice. We studied the adsorption configurations of single Cu-TCPP molecules, a sensitizer commonly used for photocatalysis, on anatase and rutile TiO2(110). Bimodal nc-AFM at room temperature and under UHV was applied to obtain high resolution on the molecules as well as on the substrate. KPFM was used to investigate the electronic properties of the adsorbed Cu-TCPP. The experimental data reveals that the Cu-TCPP molecules align themselves with respect to the substrate structure resulting in two main orientations. In both cases the KPFM showed a lowered LCPD on the sensitizer, indicating that adsorption is accompanied by charge transfer from the sensitizer to the substrate.

O 54.8 Wed 12:30 MA 004

Anchoring of a dye precursor on NiO(001) studied by non-contact atomic force microscopy — •Sara Freund[1], Antoine Hinaut[1], Nathalie Marinakis[2], Edwin C. Constable[2], Ernst Meyer[1], Catherine Housecroft[2], and Thilo Glatzel[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Department of Chemistry, University of Basel, BPR 1096, Mattenstrasse 24a, 4058 Basel, Switzerland

The properties of metal oxides can be modified when functionalized with complex molecules. These kinds of organic/inorganic surfaces have become important for enabling technologies such as hybrid photovoltaic p-type dye sensitized solar cells. A key parameter for optimized interfaces is not only the choice of the functionalization compounds but also their adsorption geometry on the substrate. The latter requires fundamental studies of such surface-molecule interactions at the nanoscale.

In this contribution, we describe the use of non-contact atomic force microscopy at room temperature to investigate the adsorption of a common organic dye precursor molecule on a NiO(001) single crystal surface. Depending on the degree of surface coverage, single molecules, groups of adsorbates with random or recognizable shapes, or even islands and domains can be identified. The interfaces were imaged with sub-molecular resolution, revealing that the dye precursor lies flat on the surface in a trans-conformation. A charge transfer from NiO to the molecular layer was observed and quantified by Kelvin probe force microscopy, only in the areas, where the molecules are closed packed.

O 54.9 Wed 12:45 MA 004

Infrared Reflection Absorption Spectroscopy Study of Phenylphosphonic Acid on Co3O4(111), CoO(111), and CoO(100) — •Matthias Schwarz, Christian Schuschke, Chantal Hohner, Thais Nascimento Silva, and Jörg Libuda — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg

We applied infrared reflection adsorption spectroscopy (IRAS) in a surface science model study under ultra-high vacuum (UHV) conditions to investigate the coverage dependent growth and thermal stability phenylphosphonic acid (d1,d2-PPA) multilayer and monolayer films on well-ordered Co3O4(111), CoO(111) and CoO(100) films on Ir(100). At 180 K, identical amorphous multilayers of intact d1,d2-PPA form on all three surfaces. They rearrange at 250 K, leading to similar recrystallized phases for all three surfaces, however with different molecular orientations. Above 340 K the multilayers desorb and only the chemically anchored monolayers remain on the surface. These are stable up to at least 550 K for all surfaces. However, surface binding and coverage dependencies in the monolayer are highly structure dependent. For d1,d2-PPA on Co3O4(111), a tridentate binding mode and full deprotonation was found for low coverages. At higher coverage, this species is replaced by partly protonated bidentate. In contrast, fully deprotonated tridentate dominates for all coverages on CoO(100). On the oxygen terminated CoO(111) bidentate species are found in the zero coverage limit. With increasing coverage, the surface restructures such that tridentate binding mode is enabled. Close to saturation, bidentate binding dominates again, presumably enabling more dense packing.

O 55: Focus Session: Structure and Chemistry of Metal-Oxide Surfaces II

Time: Wednesday 10:30–13:00 Location: MA 005

O 55.1 Wed 10:30 MA 005

Coverage-Dependent Water Agglomerates on Fe$_3$O$_4$(001): insights from theory — •Matthias Meier[1,2], Jan Hulva[1], Zdeněk Jakub[1], Jiří Pavelec[1], Martin Setvin[1], Michael Schmid[1], Ulrike Diebold[1], Cesare Franchini[2], and Gareth S. Parkinson[1] — [1]Institute of Applied Physics, Technische Universität Wien, Vienna, Austria — [2]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria

Iron oxides are used in a wide range of applications in which their surfaces interact with water. Recent studies have found significant complexity with mixed-mode adsorption and coverage dependent hydrogen bonding. This study focuses on Fe$_3$O$_4$(001) and its interaction with water. Temperature programmed desorption (TPD) and non-contact atomic force microscopy (ncAFM) are combined with density functional theory (DFT) based calculations.

Quantitative TPD spectra reveals 4 distinct peaks for the desorption of the first monolayer of water, suggesting that stable configurations of water exist. Surfaces with the in the TPD relevant water coverages were prepared and studied in a CO functionalised tip ncAFM experiment. These results will be presented in a previous talk.

DFT predicts partially dissociated dimers and trimers located on Fe cations to be found to be the most stable configurations, in-line with the known concept of cooperativity. The ring-like networks observed in ncAFM, correspond to merged trimers which are connected via additional hydrogen bonded water molecules. The formation of these features is motivated by optimizing available hydrogen bonds.

O 55.2 Wed 10:45 MA 005

cooperative formation of long-range ordering in water ad-layers on fe3o4(111) — •francesca mirabella[1], eman zaki[1], francisco ivars-barcelo[1], jan seifert[1], xiaoke li[2], joachim paier[2], joachim sauer[2], shamil shaikhutdinov[1], and hans-joachim freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Humboldt Universität zu Berlin, Berlin, Germany

Adsorption of water on magnetite surfaces has intensively been investigated on both single crystals and well-ordered epitaxial films. The initial stage of water adsorption on Fe3O4(111) surfaces remains poorly understood. In this work, we re-examined the water adsorption models on well-characterized Fe3O4(111) films, employing TPD, IRAS, and single crystal microcalorimetry. TPD data revealed sharp desorption peaks in the region 200-300 K. Each desorption peak, showing a first order kinetics, is associated with individual desorption of molecularly adsorbed water molecules having discrete adsorption energies. Both TPD and microcalorimetry results show that the desorption energy considerably decreases at increasing water coverage, from ~100 to ~50 kJ/mol. Also, combined IRAS and TPD measurements suggest that, before the formation of ASW sets in, water readily dissociates on the surface to form two hydroxyl species, involving oxygen atoms from the water itself and from the oxide surface, respectively. These species act as anchors for molecular water which self assemble into a (2x2) ordered structure. The results are rationalized by DFT in the framework of cooperative formation of the hydrogen bonding network.

O 55.3 Wed 11:00 MA 005

Water adsorption on magnetite — Francesca Mirabella[1], Eman Zaki[1], Francisco Ivars-Barcelo[1], Xiaoke Li[2], •Joachim Paier[2], Shamil Shaikhutdinov[1], Joachim Sauer[2], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut-der-Max-Planck-Gesellschaft, Berlin, Deutschland — [2]Humboldt-Universität zu Berlin, Deutschland

Fe3O4(001), well known as one of the natural growth facets of the magnetite iron oxide phase, has been recently resolved by Diebold and Parkinson. With respect to the molecular structure of water on that surface, much transferable knowledge has been generated by the pioneering work of Diebold on TiO2 as well as ZnO.

Regarding the Fe3O4(111) surface, its termination was resolved by Freund and coworkers using LEED-I/V resulting in a model with a very small R factor of 0.14. It involves a single Fe cation in its outermost atomic layer. The termination has been confirmed by a combined IRAS and DFT study using CO as a probe molecule. Recently a unique (2x2) long-range ordered structure in water adlayers on Fe3O4(111) has been studied by LEED and TPD. Upon determining relevant water ad-structures starting from 1/4 ML up to one ML coverage using DFT, the TPD can be understood. In the initial stages of H2O adsorption, individual molecules dissociate creating terminal water-related Ow-H and surface Os-H groups, serving as anchors for additional water molecules ordering via H-bonding and thus forming a (2x2) 2D structure. Adsorption energies of the modelled structures cluster in three characteristic regimes corresponding well to observed peak temperatures.

O 55.4 Wed 11:15 MA 005

Benchmarking DFT calculations for metal oxides: geometric adsorption site of copper and silver adatoms on magnetite — Matthias Meier[1,2], Zdenek Jakub[2], Jan Balajka[2], Jan Hulva[2], Roland Bliem[2], Pardeep K Thakur[3], Tien-Lin Lee[3], Cesare Franchini[1], Michael Schmid[2], Ulrike Diebold[2], Francesco Allegretti[4], •David A Duncan[3], and Gareth S Parkinson[2] — [1]University of Vienna, Vienna, Austria — [2]Technical University of Vienna, Vienna, Austria — [3]Diamond Light Source, Didcot, UK — [4]Technical University of Munich, Munich, Germany

Single-site catalysis is a promising field for studying model catalytic reactions. However, to gain true insight into the inner workings of any system, it is necessary to be able to reliably model it with theoretical calculations, and to benchmark these calculations with stringent quantitative experimental constraints. In this work we utilised X-ray standing waves (XSW) to benchmark density functional theory (DFT) calculations of one such system: single adatoms on the Fe3O4(001).

Although the clean surface structure is known [1], the geometry of the adatoms has only been probed by non-quantitative techniques, which do not provide suitable benchmarks for theoretical calculations. The surface structure of Ag and Cu adatoms was directly determined by XSW to occupy the same lateral site at a height of 0.43 Å and 0.96 Å, respectively. The commonly used DFT+U formalisations overpredicted lattice constant, but underpredicted the adatom adsorption height, raising significant questions on its applicability to this system.

[1] R. Bliem, et al., Science 346, 1215 (2014);

O 55.5 Wed 11:30 MA 005

Direct detection of Ni adatoms being driven subsurface on Fe3O4(001) — •Paul T. P. Ryan[1,2], Zdeněk Jakub[3], Jan Balajka[3], Jan Hulva[3], Roland Bliem[3], Pardeep K. Thakur[2], Tien-Lin Lee[2], Francesco Allegretti[4], David J. Payne[1], David A. Duncan[2], and Gareth S. Parkinson[3] — [1]Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ — [2]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, OX11 0QX UK — [3]Institute of Applied Physics, TU Wien, 1040 Vienna, Austria — [4]Physics Department E20, Technical University of Munich, 85748 Garching, Germany

Iron oxides are the archetypal cation defect material. For magnetite (Fe$_3$O$_4$) these cation vacancies can play an important role in its surface chemistries. Specifically, Fe$_3$O$_4$ has been observed to pattern the adsorption of a wide range of metal adatoms onto its (001) surface, where two sub-surface octahedral vacancies and one surface tetrahedral interstitial kinetically hinder the sintering of metal adatoms into nanoparticles. Despite this, STM observations of several first row transition metals, e.g. Ni and Co, suggest that these adatoms can be thermally driven into the subsurface octahedral vacancies [1]. Here we present an X-ray standing wave (XSW) study directly demonstrating the co-existence of Ni in a surface tetrahedral site, a subsurface octahedral site and a bulk octahedral site confirming the interpretation of previous STM measurements and quantitatively probing the vertical displacement of the Ni atoms at each location.

[1] R. Bliem, et al. Phys. Rev. B, 92 (2015) 075440

O 55.6 Wed 11:45 MA 005

Adsorption of formic acid on the (001) surface of Fe3O4 studied by surface x-ray diffraction — •Björn Arndt[1,2], Marcus Creutzburg[1,2], Vedran Vonk[1], Elin Graanaes[1], Konstantin Krausert[1,2], Kai Sellschopp[3], Gregor Feldbauer[3], and Andreas Stierle[1,2] — [1]Deutsches Elektron-Synchrotron (DESY) — [2]University of Hamburg — [3]Institute of Advanced Ceramics, Hamburg University of Technology

The clean (001) surface of magnetite shows a $(\sqrt{2}x\sqrt{2})$R45° surface reconstruction which gets lifted by certain adsorbates, one of them being formic acid. Although the structure of the reconstructed surface is solved with all evidence supporting the SCV model [1,2], the structure of the unreconstructed surface and the lifting mechanisms are still unknown. Formic acid allows the preparation of a nicely defined surface since it only adsorbs up to a coverage of two molecules per unit cell [3]. It also raises interest as a intermediate in the water-gas shift reaction which magnetite catalyzes, and as a model for the surface interaction of longer organic acids with magnetite. In order to get information on the structure of the surface after formic acid adsorption, we investigated it by surface x-ray diffraction measured at the ID03 beamline of the ESRF before and after dosing of formic acid. We present our results on the structure of the unreconstructed surface, compare them to DFT calculations and give insights into the lifting mechanism.

[1] Bliem, R. et al. Science. 346, 1215-1218 (2014)
[2] Arndt, B. et al. Surf. Sci. 653, 76-81 (2016)
[3] Gamba, O. et al. J. Phys. Chem. C 119, 20459-20465 (2015)

O 55.7 Wed 12:00 MA 005

Structural changes in Fe_3O_4 surfaces upon adsorption of organic acids - a DFT study — •Kai Sellschopp[1], Björn Arndt[2,3], Marcus Creutzburg[2,3], Andreas Stierle[2,3], Stefan Müller[1], and Gregor Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]DESY NanoLab, Deutsches Elektronensynchrotron, Hamburg — [3]Physics Department, Hamburg University

The structure of the major surfaces of magnetite, namely the (001) and (111) surfaces, has been a matter of debate for a long time. For the clean (001) surface the debate seems to be settled since the subsurface cation vacancy (SCV) reconstruction was found [1]. The associated $\sqrt{2}\times\sqrt{2}$ diffraction pattern changes, however, to a 1×1 pattern upon adsorption of carboxylic acids [2]. In oder to understand this structural change, we investigated the energetics of adsorption for this system and the implications for surface stability using density functional theory (DFT) calculations. Furthermore, the analysis of different adsorption sites and the electronic structure gives insight into the mechanisms of this structural change. Finally, DFT results are compared to surface X-ray diffraction (SXRD) measurements. According to our findings, adsorption of carboxylic acids may also affect the termination of the magnetite (111) surface.

[1] R. Bliem et al., *Science* **346** (6214), 1215-1218, 2014
[2] O. Gamba et al., *J. Phys. Chem. C* **119** (35), 20459-20465, 2015

Invited Talk O 55.8 Wed 12:15 MA 005

Growth and surface chemistry of rutile IrO2(110) — •Jason Weaver — University of Florida, Gainesville, FL, USA

Interest in the surface chemistry of late transition-metal oxides has been stimulated by observations that the formation of metal oxide layers tends to dramatically alter the catalytic performance of transition metals in applications of oxidation catalysis. In this talk, I will discuss our recent investigations of the growth and chemical properties of rutile IrO2 surfaces. I will discuss our studies of the oxidation of metallic Ir surfaces by O-atom beams as well as O2 at pressures above 1 Torr. We find that stoichiometrically-terminated IrO2(110) layers could only be formed by oxidizing Ir(111) and Ir(100) at sufficiently high temperature and O2 pressure. I will also discuss our recent discovery of highly facile methane and ethane activation on the IrO2(110) surface at temperatures as low as 150 K and the subsequent oxidation chemistry.

O 55.9 Wed 12:45 MA 005

Determining the structure of nitrogen doped rutile TiO2(110) — •Francesco Allegretti[1], Michael Wagstaffe[2], David A. Duncan[1,3], Tien-Lin Lee[3], Johannes V. Barth[1], Andrew G. Thomas[2], and Rob Lindsay[2] — [1]Physik-Department E20, Technische Universität München, Germany — [2]School of Materials, University of Manchester, United Kingdom — [3]Diamond Light Source, Didcot, United Kingdom

Titanium dioxide is the prototypical photocatalyst for water cracking, however its wide band gap (>3 eV) means that it only utilises a small percentage of natural sunlight. One approach to narrowing this band gap, to allow more efficient solar water cracking, is the deliberate doping of TiO2 with impurities [1]. Notably, using nitrogen as the dopant leads to a significant enhancement of the photocatalytic functionality under visible light irradiation [2]. Previous angular scanned photoelectron diffraction measurements [3] have suggested that these N3+ ions occupy O2- sites in the bulk unit cell, however the level of agreement, both between O 1s and N 1s core-level data and between theory and experiment was only qualitative. Here we present an X-ray standing wave study of N-doped rutile TiO2(110) that directly demonstrates that the majority of N3+ ions do indeed occupy O2- sites, however a minority bulk-like component with strongly different site was also observed.

[1] Z. Wang, et al., Phys. Chem. Chem. Phys. 16, 2758 (2014) [2] J. Tao, et al., J. Phys. Chem. C 118, 994 (2014) [3] M. Batzill, et al., Chem. Phys. 339, 36 (2007)

O 56: Plasmonics and nanooptics: Light-matter interaction, spectroscopy IV

Time: Wednesday 10:30–11:45 Location: MA 041

O 56.1 Wed 10:30 MA 041

Coupling of IR140 dye molecules to a plasmonic two-wire waveguide — •Christian Schörner, Subhasis Adhikari, and Markus Lippitz — University of Bayreuth, Germany

Plasmonic waveguides offer the possibility to guide light with a subwavelength confinement. For thin metal wires it is well established that they support a single fundamental waveguide mode, called TM0 mode. A combination of two such metal wires with a nanoscale gap in between results in two hybridized modes with a symmetric or antisymmetric surface charge distribution. Recent studies have been able to selectively excite these modes and detect them in the far field be means of a mode detector. Here we investigate the coupling of a near-infrared laser dye, IR140, embedded in a photoresist to such multimode plasmonic two-wire transmission lines by spatially resolved photoluminescence spectroscopy. We show that the photoluminescence of the dye molecules acts as a local source that couples simultaneously to the symmetric and antisymmetric plasmonic waveguide mode. Propagation lengths and position dependent incoupling profiles are obtained by spatially resolved excitation. We further investigate the polarization dependency of the outcoupled emission.

O 56.2 Wed 10:45 MA 041

Second harmonic generation in fully symmetric gold nanostructures — •Julian Obermeier[1], Tzu-Yu Chen[2,3], Fan-Chen Lin[4], Jer-Shing Huang[5], Chen-Bin Huang[2,3], and Markus Lippitz[1] — [1]Experimental Physics III, University of Bayreuth — [2]Institute of Photonics Technologies, National Tsing Hua University — [3]International Intercollegiate PhD Program, National Tsing Hua University — [4]Department of Chemistry, National Tsing Hua University — [5]Leibniz Institute of Photonic Technology

Higher harmonics generation in single plasmonic nanostructures is widely observed. While the third harmonic can always be generated, second harmonic generation underlies special symmetry restrictions. For common plasmonic materials as gold and silver the centosymmetric crystal structure forbids second harmonic generation in the electric dipole approximation for bulk material. Inversion symmetry can be broken by the shape of the nanostructure itself, i.e., L or V shapes. Until now this is the only known way to generate strong second harmonic signal from symmetric materials. We demonstrate an entirely new way to break the overall symmetry in structural and material fully symmetric nanostructures. The key idea is to offer an optical mode of broken symmetry in which the symmetric structure can emit. We will illustrate this effect and demonstrate experimental as well as numerical realizations.

O 56.3 Wed 11:00 MA 041

Plasmon enhanced nano-chemistry with gold nanostars — •Christian Mühlbauer[1], Wolf Knöller[1], Christioph Maier[1], Lakshmi Polavarapu[1], Theo Lohmüller[1], Jochen Feldmann[1], and Ana Huergo[2] — [1]LMU, München, Deutschland — [2]Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA), La Plata, Argentina

Plasmonic gold nanostars with radially distributed spikes display strong field enhancement at the sharptips upon excitation with light [1]. Non-radiative decay of the highly localized surface plasmons in thetip region can lead to the generation of hot-electrons that can transfer to, for example, nearbymolecules or semiconductor particles.

Here, we report on the use of gold nanostars for controlling hot-carrier induced nano-chemicalreactions. Bare gold nanostars with a core size of approximately 30 nm are synthesized in a surfactant-free approach. The stars are covered with a self-assembled monolayer of molecules that undergo areduction by electron uptake upon plasmon excitation. The efficiency and localization of this hot-carrier driven reaction is monitored and characterized by Surface Enhanced Raman Scattering (SERS).

[1] Hrelescu, T.K. Sau, A.L. Rogach, F. Jäckel, J. Feldmann; Appl. Phys. Lett. 94 (15), 153113 (2009)

O 56.4 Wed 11:15 MA 041

Two-dimensional properties of thin single-crystalline gold films — Swen Grossmann[1], •Daniel Friedrich[1], Michael Karolak[2], René Kullock[1], Enno Krauss[1], Monika Emmerling[1], Giorgio Sangiovanni[2], and Bert Hecht[1] — [1]NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany — [2]Theoretical Physics 1, University of Würzburg, Germany

Gold nanostructures such as nanowires can strongly enhance and confine optical fields while also providing excellent electronic contacts to functional elements.[1] Films of single-crystaline gold ensure well-defined experimental conditions for precision metrology and sensing.[2] In all these cases the electronic properties of gold either affect the functionality or the interpretation of experimental findings.

Here, we report notable changes in the electronic structure of gold occurring already for film thicknesses of 30nm by studying atomically flat 2D single-crystal gold platelets of variable thickness. When the gold thickness reduces below 30nm deviations from bulk electronic properties reveal themselves in a 100-fold increase of the nonlinear two-photon photoluminescence signal. Our findings are supported by density functional theory calculations and also allow us to optically resolve single-unit-cell steps.

[1] J. Kern et al., Nat Photon 9, 9 (2015)

[2] J.-S. Huang et al., Nat Comm 1, 150 (2010)

O 56.5 Wed 11:30 MA 041

Limits of Babinet principle for plasmonic antennas — •Vlastimil Křápek[1], Michal Horák[1], Martin Hrtoň[1], Andrea Konečná[2], Filip Ligmajer[1], Michael Stöger-Pollach[3], and Tomáš Šikola[2] — [1]CEITEC, Brno University of Technology, Purkyňova 123, CZ-61200 Brno, Czech Republic — [2]CIC nanoGUNE, Tolosa Hiribidea 76, E-20018 Donostia – San Sebastián, Spain — [3]USTEM, TU Vienna, Wiedner Hauptstr. 8-10, A-1040 Wien, Austria

Babinet principle relates the properties of a planar plasmonic antenna (particle) and a complemetary aperture in a thin metal film of the same size and shape. In particular, the energies of localized surface plasmon (LSP) resonances in both antennas shall be identical and the corresponding near fields shall be complementary with the electric-field distribution of the solid antenna corresponding to the magnetic-field distribution of the complementary aperture.

We investigate the limits of the Babinet principle for gold plasmonic antennas (discs and disc-shaped apertures) using electron energy loss spectroscopy, cathodoluminescence, and theoretical modeling. We show that Babinet priciple qualitatively holds but quantitative differences are found. The energies of LSP resonances in apertures are red-shifted and the near fields are less localized. Plasmonic breathing mode is observed only for particles. Observed response of apertures is stronger than that of particles, which is attributed to better heat drain and sharper edges of apertures. Finally, we discuss the possibility to employ Babinet principle for a design of electric and magnetic hot spots.

O 57: Electronic structure of surfaces: Spectroscopy, surface states II

Time: Wednesday 10:30–12:45 Location: MA 042

Invited Talk O 57.1 Wed 10:30 MA 042

Hydrogen Atom Adsorption on Surfaces Studied in Inelastic Scattering Experiments — •Oliver Buenermann — Georg-August Universität Göttingen, Germany

The first step in most reactions at surfaces is the adsorption of the reactants. For this to happen their translational and binding energy have to be dissipated to the solid. In inelastic scattering experiments, adsorption can be studied on model systems in great detail. Based on such experiments new theoretical models can be developed that accurately describe the delicate interplay between electronic and nuclear motion in prototypical chemical reactions. Hydrogen adsorption is of special interest, as the small mass of the atoms leads to an inefficient phonon coupling, but sticking probabilities on surfaces can still be high.

Recently, we could show that in case of H-atom scattering from Au(111) a large amount of the translational energy can be transferred to electronic excitation of the metal [1]. We expanded our studies to various surfaces including a set of metals, insulators, and graphene. Furthermore, the influence of the projectile mass was investigated by replacing hydrogen by its heavier isotope deuterium. The experimentally observed dependencies are presented and their implication for the underlying energy transfer processes are discussed.

[1] Bünermann, O. et al., Science 350, 1346-1349 (2015).

O 57.2 Wed 11:00 MA 042

Work function measurements on heterogeneous surfaces: The role of electrostatic potentials for ultraviolet photoelectron spectroscopy (UPS) — •Thorsten Schultz[1], Thomas Lenz[2], Naresh Kotadiya[2], Georg Heimel[1], Gunnar Glasser[2], Rüdiger Berger[2], Paul W. M. Blom[2], Patrick Amsalem[1], Dago M. de Leeuw[2], and Norbert Koch[1] — [1]Humboldt Universität zu Berlin, 12489 Berlin — [2]Max Planck Institute for Polymer Research, 55128 Mainz

UPS is a primary technique to determine the work function of surfaces. According to literature, heterogeneous surfaces are expected to exhibit one secondary electron cut-off (SECO) representing an area-averaged work function. However, several reports show that more than one cut-off can be observed for heterogeneous surfaces. To clarify this discrepancy, heterogeneous model surfaces consisting of bilinear arrays, providing a work function contraast of more than 1 eV, were investigated. With UPS we measure two SECOs, one reflecting the high work function surface fraction and the other an averaged work function. The electrostatic potential away from the surface was measured by Kelvin-probe force microscopy and compared to electrostatic modeling. With this we can quantitatively explain that the high work function areas lead to an additional energy barrier for electrons emitted from the low work function areas.[1] We detail the role of experimental parameters on the appearance of SECOs and how this influences the determination of ionization energy of molecules deposited on heterogeneous surfaces. [1] T. Schultz et. al, Adv. Mat. Interf. 4, 1700324 (2017)

O 57.3 Wed 11:15 MA 042

1,3-Di(methoxy)imidazolium ionic liquid mixtures investigated by angle-resolved X-ray photoelectron spectroscopy — •Bettina Heller[1], Claudia Kolbeck[1], Inga Niedermaier[1], Sabine Dommer[2], Jürgen Schatz[2], Hans-Peter Steinrück[2], and Florian Maier[2] — [1]Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Germany — [2]Lehrstuhl für Organische Chemie I, FAU Erlangen- Nürnberg, Germany

Ionic liquids (ILs) - salts with melting points typically well below 100 °C and an extremely low vapour pressure - allow for applying surface science methods under UHV condition such as X-ray photoelectron spectroscopy (XPS). In this work, the functionalised IL 1,3-di(methoxy)imidazolium hexafluorophosphate ([(MeO)2Im][PF6])[1] and its mixtures with two non-functionalised 1,3-dialkylimidazolium ILs, namely 1-methyl-3-octylimidazolium bis[(trifluoromethyl)sulfonyl] imide ([C8C1Im][Tf2N]) and 1,3-diethylimidazolium hexafluorophoshate ([C2C2Im][PF6]), were investigated. We were using our Dual Analyser System for Surface Analysis (DASSA)[2] for simultaneous measurements in 0° (bulk sensitive) and 80° (surface sensitive) emission relative to the surface normal of the sample. Changes in the angle-resolved XP spectra directly reveal differences in surface and bulk composition of the mixtures, whereas pronounced differences in the electronic structure due to functionalisation are reflected in large chemical shifts.

[1] G. Laus et al., Z. Naturforschung 2007, 62b, 295-308.

[2] I. Niedermaier et al., Rev. Sci. Instrum. 2016, 87, 045105.

O 57.4 Wed 11:30 MA 042

A three electrodes electrochemical setup for XPS studies in ionic liquids — •Francesco Greco, Radha Gobinda Bhuin, Hans-Peter Steinrück, and Florian Maier — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (ILs) are widely used in electrochemical studies due to their large electrochemical window, good ionic conductivity and thermal stability. These properties together with their extremely low vapor pressure make them unique candidates to perform electrochemistry in liquid media in combination with ultra-high-vacuum-based surface science techniques. In this work, a three electrodes electrochemical cell for X-ray-Photoelectron-Spectroscopy (XPS) studies has been developed, which allows in-situ cyclic voltammetry and chronoamperometry using the molybdenum sample holder as counter electrode, a platinum wire as quasi-reference electrode and a wire of chosen material as working electrode. The experiments are performed in a "Dual Analyzer System for Surface Analysis (DASSA)"[1] which enables angle-resolved X-ray Photoelectron Spectroscopy (ARXPS) using two electron analyzers mounted for simultaneous measurements in 0° (bulk-sensitive) and 80° (surface-sensitive) emission relative to the surface normal.

F.G., R.G.B. and H.P.S. thank the ERC for financial support through an Advanced Investigator Grant to H.P.S.!

[1] I. Niedermaier, C. Kolbeck, H.-P. Steinrück, F. Maier, Rev. Sci. Instrum. 87 (2016) 045105

O 57.5 Wed 11:45 MA 042

Correction and Suppression of the Space-Charge Effect in Cathode-Lens Microscopes — •Benedikt Schönhense[1], Katerina Medjanik[2], Dmitry Vasilyev[2], Sergey Babenkov[2], Martin Ellguth[2], Hans-Joachim Elmers[2], and Gerd Schönhense[2] — [1]Imperial College London, UK — [2]56

Previous pump-and-probe photoemission experiments have revealed that the Coulomb interaction in the pulsed beam (commonly referred to as "space-charge problem") is a serious obstacle, in particular due to background electrons released by the pump pulse [1]. Theoretical work [2] has uncovered the reason for the dramatic deterioration of the imaging performance in conventional cathode lenses (PEEMs, k-microscopes): All slow electrons are efficiently focused into the lens column where they travel along the optical axis and exert strong forces on the primary photoelectrons. Shifts up to 10 eV have been measured at the conditions of beamline P04 of PETRA III. We present strategies of an a-posteriori correction of the Lorentzian deformation of the momentum distributions [2] and of an a-priori suppression of the deterministic part of Coulomb interaction by "extraction-field tailoring".

[1] L.-P. Oloff et al., J. of Appl. Phys. 119, 225106 (2016)

[2] B. Schönhense et al., New J. Phys., under review

O 57.6 Wed 12:00 MA 042

On multi-electron emission from surfaces — Iuri S. Brandt, Zheng Wei, Jürgen Kirschner, and •Frank O. Schumann — Max-Planck Institut für Mikrostrukturphysik, Halle, Germany

We have studied the electron pair emission process from surfaces due to the impact of a primary positron. The existence of this process implies a two-step scattering event. In the first step the primary positron scatters with a valence band electron. Each particle of the positron-electron pair can collide with another valence electron. We find that the electron pair intensity is on the same scale as the positron-electron pair intensity. This suggests that a significant contribution of the pair intensity is actually due to the emission of three particles. Our instrument is only able to detect two particles in coincidence. We also observe a strong material dependence of the coincidence intensity. In previous studies with primary electron excitation or photon absorption we observed that NiO displays the highest coincidence rate.[1,2] The same observation we have made in this work. We find that NiO has a factor of 3 higher coincidence intensity compared to the Ag(100) substrate. We also note that the pair intensity scales with the single electron rate. The higher the singles rate the higher the coincidence rate. We discuss the fact that very different excitation processes leading to pair emission give similar results.

[1] I.S. Brandt et al., Phys. Rev. B 92, 155106 (2015).

[2] F.O. Schumann et al., Phys. Rev. B 93, 235128 (2016).

O 57.7 Wed 12:15 MA 042

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

In systems with spin-orbit coupling (SOC) and electronic correlations of comparable strength, like Pb/Si(557), a Spin-Orbit-Density-Wave is formed at low temperatures resulting in an insulating state below 78K [1]. It is characterized by Rashba-type spin-split bands with nesting between opposite helical states at the Fermi surface.

For Si(111) covered by 0.3 ML Sn, a $\sqrt{3}\times\sqrt{3}$ reconstruction is formed which shows a Mott-type Metal-insulator transition upon cooling below 70 K [2]. Recently, this system was investigated by ARPES and DFT suggesting a collinear antiferromagnetic order with a $2\sqrt{3}\times\sqrt{3}$ spin cell at low temperatures [3].

Spin-resolved ARPES measurements reveal the existence of a spin-ordered surface unit cell larger than $\sqrt{3}\times\sqrt{3}$. However, the SOC induced effects are small, thus the insulating state is mainly governed by electronic correlation effects.

[1] C. Brand et al., Nat. Comm. **6**, 8118 (2015).

[2] S. Modesti et al., PRL **98**, 126401 (2007).

[3] G. Li et al., Nat. Comm. **4**, 1620 (2013).

O 57.8 Wed 12:30 MA 042

Fermi Surface, Fermi-Velocity and Circular Dichroism of Rhenium Measured with Soft X-Rays — •Katerina Medjanik[1], Dmitry Vasilyev[1], Sergey Babenkov[1], Martin Ellguth[1], Benedikt Schönhense[2], Jens Viefhaus[3], Hans-Joachim Elmers[1], and Gerd Schönhense[1] — [1]JGU, Inst. für Physik, Mainz — [2]Imperial College London, UK — [3]DESY Photon Science, Hamburg

Parallel-imaging k-space microscopy with time-of-flight energy recording has substantially advanced photoemission data recording. In combination with the circularly-polarized high-brilliance soft X-rays at beamline P04 at PETRA III (Hamburg), we acquired 4D photoemission data arrays $I(E_B,k_x,k_y,k_z)$ for both photon helicities in the full bulk Brillouin zone and energy range of the d-band complex. Here, we present the experimental Fermi surface map for rhenium (hcp), revealing unprecedented detail quality. The full data set, including Fermi-velocity distribution $v_F(\boldsymbol{k})$ and circular dichroism texture have been obtained in a few hours of acquisition time. Maximum k_z-resolution has been achieved by variation of the photon energy in small steps. Data are compared with our previous results for tungsten (bcc) [1] and iridium (fcc) [2].

[1] K. Medjanik et al., *Nat. Materials* **16**, 615 (2017); [2] G. Schönhense et al., *Ultramicr.* **183**, 19 (2017).

O 58: 2D materials beyond graphene: TMDCs, silicene and relatives II

Time: Wednesday 10:30–13:00 Location: MA 043

O 58.1 Wed 10:30 MA 043

Fabrication of germanane from Ge(111) single-crystal wafers — •Kornelia Huba[1], Ulrich Hagemann[2], and Hermann Nienhaus[1] — [1]Faculty of Physics, CENIDE, University of Duisburg-Essen, Duisburg — [2]Interdisciplinary Center for Analytics on the Nanoscale (ICAN), CENIDE, Duisburg

Germanane is a layered semiconducting material composed of single two-dimensional Ge sheets with dangling bonds saturated with hydrogen atoms. It is fabricated in a two-step procedure from clean Ge(111) wafers. First, a Zintl phase of CaGe$_2$ is formed under ultrahigh vacuum conditions by evaporating Ca atoms onto Ge at 810°C. Second, the sample is transferred under atmosphere to the wet-chemical treatment where it is etched in concentrated hydrochloric acid (HCl) at low temperatures for several hours. This leads to deintercalation of Ca and forming layered germanane flakes on top of the Ge(111) substrate. The flakes are exfoliated and transferred to other substrates, e.g., Si wafers for characterisation. The lateral extension of the germanane flakes ranges between 30 and 150 μm. X-ray photoelectron spectroscopy for chemical analysis detects Ge, no Ca and slight oxygen contaminations. From a 20% attenuation of the Si substrate line intensities a germanane layer thickness in the nm range is extracted demonstrating that single layer preparation is feasable. Currently, transmission electron microscope studies and micro-Raman spectroscopy are performed to elucidate morphology and structure of the germanane material.

O 58.2 Wed 10:45 MA 043

On the adatom doping of 2-Dimensional siligene (SiGe) with alkali metals — •Amretashis Sengupta — BCCMS, University of Bremen, Am Fallturm 1, 28359 Bremen, Germany — Indian Institute of Engineering Science and Technology, Shibpur, Howrah - 711 103, India

An interesting hybrid 2D material, siligene has received attention for its possible applications in nanoelectronics and thermoelectrics. In this work we study the effect of adatom doping of 2D SiGe with alkali metal atoms (Li, Na and K), with density functional theory (DFT) simulations using generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof(PBE) functionals. The simulations showed a moderate adsorption energy of 0.75, 0.62 and 0.87eV for Li, Na and K atoms respectively, with possible doping concentrations upto M$_{0.88}$SiGe (M=Li,Na,K). For ion-battery applications, the specfic capacites are evaluated as 223, 196 and 175 mAhg^{-1} for Li,Na and K storage respectively. Nudged elastic band (NEB) simulations showed a diffusion barrier of 0.71, 0.49 and 0.32eV for Li, Na and K atoms. In all cases a significant modulation in the Fermi energy (E$_f$) could be seen for varying degrees of doping. While Li adatom can dope the system from slight p-type to n-type (δE$_f$=-0.05 to +0.5), the Na and K atoms dope the system from moderate to strongly n-type (δE$_f$=+0.3 to +1.4 for Na and +0.6 to +1.86 for K) depending upon coverage. The results show possibilities concerning applications of 2D SiGe in ion-batteries, sensors and nanoscale devices.

O 58.3 Wed 11:00 MA 043

Unoccupied band structure of Si nanoribbons on Ag(110) — •Nils Fabian Kleimeier[1,2], Gabi Wenzel[1], Adrian Joe Urban[1], Jürgen Braun[3], Hubert Ebert[3], Elena Voloshina[4], Yuriy Dedkov[4], and Helmut Zacharias[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster — [2]Center for Soft Nanoscience (SoN), Westfälische Wilhelms-Universität Münster — [3]Department Chemie, Ludwig-Maximilians-Universität München — [4]International Centre for Quantum and Molecular Structures, Shanghai University

Adsorption of Si atoms on the Ag(110) surface leads to the formation of monolayer silicon nanoribbons along the [$\bar{1}$10] direction. Depending on the surface temperature during adsorption, nanoribbons with widths of either 0.8 nm or 1.6 nm, as determined by STM, are formed, leading to a (3 × 2) or (5 × 2) reconstruction, respectively. Employing k-resolved inverse photoemission spectroscopy (KRIPES), the unoccupied band structure of both reconstructions has been determined and is compared to measured and calculated KRIPES spectra of the bare Ag(110) surface. The experimental results for the band structures of both nanoribbon types are compared to DFT calculations for different pentagonal as well as hexagonal silicon nanoribbon models on Ag(110) found in the literature. As expected for one-dimensional materials, all states associated with the nanoribbons show no dispersion in the $\overline{\Gamma Y}$ direction (across the nanoribbons), but disperse in $\overline{\Gamma X}$ direction (along the nanoribbons).

O 58.4 Wed 11:15 MA 043

STM Study of Current-Induced Forces in Graphene Nanoribbons on Au(111) — •Tobias Preis[1], Sasha Vrbica[2], Nemanja Kocic[1], Ulrike Paap[1], Jonathan Eroms[1], Dieter Weiss[1], Jan van Ruitenbeek[2], and Jascha Repp[1] — [1]Universität Regensburg, Institut für Experimentelle und Angewandte Physik - Regensburg, Germany — [2]Leiden University, Huygens-Kamerlingh Onnes Laboratorium - Leiden, Netherlands

In electromigration, an electrical current flowing through a material exerts a force on atoms in the material or on its surface eventually leading to a displacement of these atoms. Although this phenomenon is technologically relevant for device reliability and has been addressed both theoretically [1] and experimentally [2] it is not fully understood yet. Electromigration of single gold atoms on a Ni(111) surface was reported based on scanning tunneling microscopy (STM) experiments [3].

Here, we address this issue with a very similar approach as in [3] but for single cobalt atoms adsorbed on narrow graphene nanoribbons adsorbed on a metal surface. By approaching the ribbons with an STM tip and injecting current pulses we observe motion of the adatoms predominantly along the ribbons. We could not observe a preferential direction with respect to a motion towards versus away from the tip.

[1] P. J. Rous et al., Phys. Rev. B 62, 8478-8486 (2000)
[2] B. C. Regan et al., Nature 428, 924-927 (2004)
[3] K.-F. Braun et al., Appl. Phys. Lett. 90, 023118 (2007)

O 58.5 Wed 11:30 MA 043

Thermal transport in 2D transition metal dichalcogenides within the relaxon picture — •Michele Simoncelli[1], Andrea Cepellotti[2,3], and Nicola Marzari[1] — [1]Theory and Simulations of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Station 12, CH-1015 Lausanne, Switzerland. — [2]Department of Physics, University of California at Berkeley, California 94720, USA — [3]Materials Science Division, Lawrence Berkeley National Laboratory, California 94720, USA

In electronics, the contemporary quest for device miniaturization has stimulated the search for 2D semiconducting materials with direct band-gap and favorable mechanical properties. Moreover, electronic devices are subject to Joule heating, which can result in a temperature increase up to values that cause chip damages or even melting. It is therefore desirable to find materials featuring a high thermal conductivity to ease the heat removal. In this study we focus on the thermal transport in 2D transition metal dichalcogenides (TMDCs), which are promising materials for their electronic and mechanical properties.

It has been shown recently [Cepellotti and Marzari, PRX, 2016] that the microscopic mechanism underlying heat conduction in crystals can be explained in terms of a gas of collective phonon excitations, called relaxons and defined as the eigenvectors of the scattering matrix appearing in the phonon Boltzmann equation. We used this theoretical framework to predict the thermal properties of the TMDCs of type MX$_2$, where M=Mo, W and X=S, Se, Te.

O 58.6 Wed 11:45 MA 043

The Role of Substrate Symmetry on the Structural Properties of 2D Materials — •Antonio J. Martínez-Galera and José M. Gómez-Rodríguez — Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

Predicting the properties that graphene and h-BN monolayers will exhibit after their growth on a certain substrate is a major challenge. While the influence on these properties of the electron configuration of the atoms comprising the underlying surface is well-known, the effects of substrate geometry still remain unclear. Herein, the structural properties of h-BN and of graphene monolayers grown on the rectangularly-packed Rh(110) surface are characterized and compared to those that both materials exhibit on substrates with different crystallographic orientations. The STM apparent corrugation of the quasi-one-dimensional moiré patterns found in both systems is unexpectedly small, compared to the values previously reported for a number of lattice-mismatched interfaces with hexagonal supports of 4d metals, in which, as in the case of Rh, the d band is half-filled and, as a result, a strong interaction of the 2D material layer with the substrate is expected. This discrepancy is explained by the differences in the possible binding landscapes at the interface for differently oriented substrates. In consequence, a rule is derived to predict how the corrugation at the interface, as well as the existence and the extent of sub-regions, within the moiré supercell, containing favorable sites for orbital mixing between h-BN or graphene and their supports depend on the substrate symmetry.

O 58.7 Wed 12:00 MA 043

Damage Mechanisms in Two-Dimensional Materials — Silvan Kretschmer[1] and •Arkady V. Krasheninnikov[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Applied Physics, Aalto University School of Science, Aalto, Finland

As the influence of defects on material properties heavily depends on the dimensionality, understanding defect production mechanisms in detail plays a major role for two-dimensional (2D) materials. The defect production under irradiation e.g. in the transmission electron miscroscope (TEM) can be subdivided into three mechanisms, namely knock-on damage, ionization damage and chemical etching. Surprinsingly, as shown for transition metal dichalcogenides, in TEM defects are produced far below the knock-on threshold [1]. Here we investigate ionization and excitation damage mechanisms for Graphene, MoS_2 and hexagonal BN using first-principles simulation techniques.

[1] Y.Lin, T.Björkman, H.Komsa et al. *Nature Communications* **6** (2015), 6736.

O 58.8 Wed 12:15 MA 043

Observing structural information of TMDCs with FM-AFM in ambient and UHV — •Korbinian Pürckhauer, Dominik Kirpal, Leo Waldhauser, Alfred J. Weymouth, and Franz Giessibl — University of Regensburg, Regensburg, Germany

The development in nanoelectronics demands reducing the size of its elements which led to an increase of interest in TMDCs. These show a range of interesting properties like a band gap in the range of Si and GaAs and allow high on/off switching ratios for FETs.

We studied bulk MoS_2, WS_2, $MoSe_2$ and WSe_2 cleaved in air with a qPlus AFM. The high stiffness ($k > 1\,\mathrm{kN}$) of the qPlus sensor allows us to operate in the frequency-modulation mode with sub-Angstrom amplitudes. On all surfaces we were able to observe atomic resolution in ambient conditions. The spacing between steps on MoS_2 and WS_2 were very large (at least hundreds of nm). In contrast, the $MoSe_2$ and WSe_2 surfaces appeared to be contaminated directly after cleavage. Both surfaces were covered with particles that were approximately 10 nm high. These particles were not observed on the MoS_2 and WS_2 surfaces. Transferring $MoSe_2$ into vacuum and annealing at 700°C resulted in a cleaner surface. This suggests that TMDCs with Sulfur as a chalcogen atom are more suitable for devices made in ambient conditions.

O 58.9 Wed 12:30 MA 043

Lateral heterostructures of two-dimensional materials by electron-beam induced stitching — •Andreas Winter[1], Antony George[1], Christof Neumann[1], Zian Tang[1], Michael Mohn[2], Johannes Biskupek[2], Nirul Masurkar[3], Arava Reddy[3], Thomas Weimann[4], Uwe Hübner[5], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm — [3]Department of Mechanical Engineering, Wayne State University, 48202 Detroit, USA — [4]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig — [5]Leibniz Institute of Photonic Technology, 07745 Jena

We present novel two-dimensional (2D) lateral heterostructures of graphene and MoS_2 sheets with molecular carbon nanomembranes (CNMs), synthesized by electron beam induced stitching. Graphene and MoS_2 were transferred onto gold substrates and lithographically patterned. Self-assembled monolayers (SAMs) of aromatic thiols were grown in the areas between the 2D materials. Irradiation with an electron beam converts the SAMs into CNMs and simultaneously stitches the CNM to graphene or MoS_2, forming a heterogeneous film of two different materials. These heterostructures are mechanically stable, enabling their preparation as freestanding sheets. We characterized them by means of Raman spectroscopy, atomic force microscopy (AFM), helium ion microscopy (HIM), X-ray photoelectron spectroscopy (XPS) and high resolution transmission electron microscopy (HRTEM) and find that they possess molecularly sharp boundaries.

O 58.10 Wed 12:45 MA 043

Low energy electron induced crosslinking of aromatic SAMs — •Christof Neumann[1], Richard A. Wilhelm[2,3], Maria Küllmer[1], Andreas Winter[1], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Institute of Applied Physics, TU Wien, 1040 Vienna, Austria — [3]Institute of Ion Beam Physics and Materials Research, HZDR, 01328 Dresden, Germany

Aromatic self-assembled monolayers (SAMs) can be converted into carbon nanomembranes (CNMs) via low energy electron irradiation [1]. Due to their mechanical and thermal stability as well as tunable chemical functionalization, CNMs are a 2D material with a large potential for application. Nevertheless, the conversion process is not yet understood in detail on the molecular level. In order to study the crosslinking we subsequently irradiated 4'-nitro-4-biphenylthiol SAMs on gold/mica substrates with different electron energies (5-50 eV) in UHV. Here we present the results obtained under in-situ conditions using X-ray photoelectron spectroscopy (XPS), Low Energy Electron Diffraction (LEED) and Low Energy Electron Microscopy (LEEM). To show the successful conversion process the samples were transferred onto TEM grids and Si wafers with 300 nm of thermal oxide and analyzed using optical, scanning electron (SEM) and atomic force microscopy (AFM). [1] A. Turchanin and A. Gölzhäuser, Adv. Mater. 28, 5075 (2016)

O 59: Nanostructures at surfaces: 1D and 2D structures and networks I

Time: Wednesday 10:30–13:00 Location: MA 141

O 59.1 Wed 10:30 MA 141

Physical Vapor Deposition at Oblique Angles — •Christoph Grüner, Susann Liedtke, and Bernd Rauschenbach — Leibniz Institute of Surface Engineering (IOM), Permoserstraße 15, D-04318 Leipzig, Germany

Physical vapor deposition at oblique angles is an often found circumstance in applied thin film deposition. Besides the geometric relation between material source and the substrate, the topography of the substrate as well as its curvature, shape and roughness locally lead to oblique deposition. Thin films deposited at oblique angles can show significant morphological differences compared to the vertically deposited counterparts. The formation of porous films, consisting of a large number of tilted columns is typically observed under non-normal deposition conditions. Deposition at highly oblique angles is also utilized to create separated nanostructures on surfaces. Techniques referring to this are known as oblique angle deposition (OAD) and glancing angle deposition (GLAD). Although these techniques have been used since the 1950s, a model that is able to adequately predict the properties of the obliquely grown films has not been found yet. In this contribution, a model is proposed, which allows predicting the density, growth speed and columnar tilt angle of obliquely deposited thin films for different materials over the complete angle of incidence range.

O 59.2 Wed 10:45 MA 141

Texture, morphology and microstructure of nanostructured Ti thin films grown by oblique angle deposition — •Susann Liedtke, Christoph Grüner, Jürgen W. Gerlach, Andriy Lotnyk, and Bernd Rauschenbach — Leibniz Institute of Surface Engineering (IOM), Permoserstraße 15, D-04318 Leipzig, Germany

Highly porous, sculptured metallic thin films are interesting for numerous applications such as electrodes in fuel cells and Li-ion batteries as well as for surface enhanced Raman sensors. Combining electron beam evaporation and oblique angle deposition (OAD) represents a powerful method to sculpture such thin films consisting of separated, tilted nano-sized columns. Tailoring the properties of the thin films requires the ability to control the shape of the nano-sized columns precisely. Although considerable research has been performed on insulating and semi-conducting OAD-structures, the growth of metallic OAD-structures still remains only fragmentarily understood. However, it is known that the angle of the incoming particle flux θ and the substrate temperature T influence the growth of such columns significantly. The experimental setup allows covering a substrate temperature range between 77 K $<$ T $<$ 1000 K, while the angle of the incoming particle flux can be varied between $0^\circ < \theta < 90^\circ$. The presentation focuses on the texture, morphology and microstructure of Ti porous thin films depending on these parameters. The samples were deposited on natively and thermally oxidized Si(100) substrates. Analysis was carried out using X-ray diffraction in-plane pole figure measurements, scanning electron microscopy and transmission electron microscopy.

O 59.3 Wed 11:00 MA 141

Cobalt silicide nanostructures on planar and vicinal Si(111) surfaces — •Lars Freter, Martin Franz, Stephan Appelfeller, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

The growth of transition metal silicides on Si(111) surfaces is interesting since they form various different nanostructures. Using Co is especially promising because Co silicide nanostructures range from small ring clusters over two-dimensional reconstructions, like the Si(111)$\sqrt{7} \times \sqrt{7}$R19.1°-Co and the Si(111)$\sqrt{13} \times \sqrt{13}$R13.9°-Co, to three-dimensional islands and nanowires consisting of bulk silicides.

Here, the properties of these structures were investigated using scanning tunneling microscopy and spectroscopy as well as low energy electron diffraction. The samples were prepared using Co coverages between submonolayers and some monolayers and temperatures between 500 °C and 900 °C.

In order to force the formation of Co silicide nanowires instead of planar films, the vicinal Si(557) and Si(553) surfaces were also employed. Here, the formation of elongated, nanowire-like silicide islands is observed.

O 59.4 Wed 11:15 MA 141

Pressure-induced melting of confined ice — •Kai Sotthewes[1,2], Pantelis Bampoulis[1,3], Harold Zandvliet[1], Detlef Lohse[3], and Bene Poelsema[1] — [1]Physics of Interfaces and Nanomaterials, Mesa+ Institute of Nanotechnology, University of Twente, P.O. Box 217, 7500AE Enschede, The Netherlands — [2]II. Institute of Physics B and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany — [3]Physics of Fluids Group and Max Planck Center Twente, University of Twente, P.O. Box 217, 7500AE Enschede, The Netherlands

The states of aggregation of confined water are highly important and of great fundamental interest in surface chemistry, life and environmental sciences. Due to limited experimental access, a coherent understanding of the phase behavior and the occurring phase transitions of interfacial ice is still lacking. Using scanning probe techniques, we studied the fully reversible ice-liquid water transition for water confined between graphene and muscovite mica. A transition from two-dimensional (2D) ice into a quasi-liquid phase is observed by applying a pressure exerted by an atomic force microscopy (AFM) tip. At room temperature the critical pressure amounts to about 6 GPa. The transition is completely reversible: refreezing occurs when the applied force is lifted. The critical pressure to melt the 2D ice decreases with temperature and the latent heat of fusion is 0.15 eV/molecule, being twice as large as for bulk ice. Our findings form a paradigm of the classic phenomenon of regelation decoupled from environmental thermal effects.

O 59.5 Wed 11:30 MA 141

Topological states and nearly flat electron band in engineered atomic lattices — •Robert Drost[1,2], Ari Harju[1], Teemu Ojanen[1], and Peter Liljeroth[1] — [1]Aalto University School of Science,Espoo, Finland — [2]Max-Planck-Institut for Solid State Research, Stuttgart, Germany

Topological materials exhibit protected edge modes that have been proposed for applications in spintronics and quantum computation. Although a number of such systems exist, it would be desirable to be able to test theoretical proposals in an artificial system that allows precise control over key parameters of the model. The essential physics of several topological systems can be captured by low-dimensional tight-binding models which can also be implemented in artificial lattices. Here, we apply this method using a vacancy lattice in a chlorine monolayer on Cu(100). We use low-temperature scanning tunnelling microscopy to fabricate such lattices with atomic precision and probe the resulting local density of states. We implement of two tight-binding models of fundamental importance: the polyacetylene (dimer) chain with topological domain-wall states, and the Lieb lattice with a flat electron band. These results provide an important step forward in the ongoing effort to realize designer quantum materials with tailored properties.

O 59.6 Wed 11:45 MA 141

Exchanging the central metal atoms in adsorbed macrocycles — •Alexandra Rieger[1], Stephan Schnidrig[2], Benjamin Probst[2], Karl-Heinz Ernst[1], and Christian Wäckerlin[1] — [1]Swiss Federal Laboratories for Material Science and Technology, Dübendorf, Switzerland — [2]University of Zurich, Switzerland

Surface adsorbed macrocycles exhibit a number of interesting physical and chemical properties, many of them are determined by their transition metal centers. We report on the substitution of the transition metals in surface-adsorbed pyrphyrin (P), a porphyrin-related macrocycle. Using scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS), we demonstrate a defined hierarchy in this replacement process, that is: Ni substitutes Cu, Fe substitutes Cu and Fe substitutes Ni, although less efficiently. The Cu to Ni and Cu to Fe atom replacement reactions are surprisingly efficient and proceed completely at 423 K. These results open up new possibilities to study coordination chemistry in solvent free environment. Furthermore, we show that the atomic hydrogen produced by on-surface metalation can lead to the scision of the cyano groups on the rim of the macrocycle which desorb as hydrogen cyanide. This result implies that atomic hydrogen, which is produced in numerous on-surface reactions, can induce interesting reactions.

O 59.7 Wed 12:00 MA 141

Identification and Nanoengineering of Hot Electron-Induced Tautomerization — •Jens Kügel[1], Markus Leisegang[1], Markus Böhme[1], Andreas Krönlein[1], Aimee Sixta[2], and Matthias Bode[1,3] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]University of Texas at Austin, Austin, Texas 78712, United States — [3]Wilhelm Conrad Röntgen Center of Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg

The tautomerization of molecules, that is, the bistable position of hydrogen protons within an organic frame, has recently been discussed as a potential avenue toward nanoscale switches. Whereas consensus exists that STM-induced local switching is caused by inelastic electrons that excite vibrational molecular modes [1], the detailed process responsible for nonlocal switching and methods to control this process are largely unknown. Here, we demonstrate for dehydrogenated H_2Pc molecules on Ag(111) how to controllably decrease or increase the probability of nonlocal, hot electron-induced tautomerization by Ag nanostructures [2]. We will show that Ag atom walls act as potential barriers that exponentially damp the hot electron current between the injection point and the molecule. Furthermore, by using elliptical nanostructures, we could coherently focus hot electrons onto the molecule, resulting in an almost tripled switching probability.

[1] T. Kumagai *et. al.*, Phys. Lett. **111**, 246101 (2013)

[2] J. Kügel *et. al.*, Nano Lett. **17**, 5106 (2017)

O 59.8 Wed 12:15 MA 141

Below 2D: Design and characterization of electronic fractals — •Marlou Slot[1], Sander Kempkes[2], Saoirsé Freeney[1], Stephan Zevenhuizen[1], Daniel Vanmaekelbergh[1], Ingmar Swart[2], and Cristiane Morais Smith[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, Netherlands — [2]Institute for Theoretical Physics, Utrecht University, Netherlands

The dimensionality and geometry of a quantum system are decisive factors for its electronic properties. So far, research has focused on systems with integer dimensions, ranging from 0D to 3D. However, very little is known about the properties of electrons in fractional dimensions. This is because geometric fractals, although pervasive in our everyday life, remain elusive in the quantum world. One possible route to create electronic quantum fractals is by confining the surface state electrons of Cu(111) by accurate positioning of adsorbed CO molecules [1,2]. Here, we realize and characterize an electronic Sierpiński triangle fractal with dimension 1.58. Using scanning tunneling spectroscopy and wave-function mapping, we observe single-electron wave functions with a fractal dimension derived from the Sierpiński geometry. These results bear importance for the understanding of the transport properties of and charge storage in fractal-like structures, opening the path to fractal-dimension electronics in a systematic and controlled manner.

1. K.K. Gomes *et al.*, Nature 483, 306-310 (2012)
2. M.R. Slot *et al.*, Nature Physics 13, 672-676 (2017)

O 59.9 Wed 12:30 MA 141

Regulation of Organic Structures by Cations and Anions from Salts — •Lei Xie and Wei Xu — Interdisciplinary Materials Research Center, Tongji-Aarhus Joint Research Center for Nanostructures and Functional Nanomaterials College of Materials Science and Engineering, Tongji University Shanghai 201804 (P.R. China)

From the combination of STM imaging and DFT calculations, we show that both cations and anions provided by salts can simultaneously interact with different sites of the target molecules resulting in structural formation in a synergistic way. In the first example, we choose the 9-ethylguanine molecule (9eG) and transition metal halides as model system, showing that metal-organic structures can further be stabilized by the electronic interactions between halogen anions and hydrogen-rich sites of molecules. In the second case, 1-methylcytosine (1mC) and alkali halide are chosen where both ions participating in structural formation. The elementary metal*organic motifs are connected by Cl in a variety of fashions demonstrating structural diversity. These findings provide a facile method of introducing both cations and anions at the same time for the regulation of organic structures.

References: [1] L. Xie, C. Zhang, Y. Ding, W. Xu*, Angew. Chem. Int. Ed. 56, 5077-5081, 2017 [2] L. Xie, C. Zhang, Y. Ding, W. E, W. Xu*, Chem. Commun. 53, 8767-8769, 2017

O 59.10 Wed 12:45 MA 141

Large area nanopatterns in elastomers by nanosphere mask replication — •Julius Bürger[1], Katharina Brassat[1], Thorsten Meyers[2], Ulrich Hilleringmann[2], and Jörg K. N. Lindner[1] — [1]Paderborn University, Dept. of Physics, Paderborn, Germany — [2]Paderborn University, Sensor Technology Dept., Paderborn, Germany

Soft lithography is a well-established low-cost surface patterning technique using structured elastomers for transferring large-scale patterns with nanometer-sized features. The biocompatible, optically transparent, highly flexible and isolating polydimethylsiloxane (PDMS) is a widely used elastomer which can be poured on a mold. After cross-linking it is released by a peel off, replicating the surface morphology of the mold. For the creation of a mold with nanoscale features, we exploit nanosphere lithography (NSL). In NSL a colloidal suspension forms a hexagonally close packed sphere mask on a substrate by self-organization. The sphere diameter can range from nanometers to several micrometers and post sphere deposition treatments of the masks such as plasma shrinking yield a huge diversity of possible masks. We use a monolayer of 618 nm polystyrene spheres on a silicon substrate as a mold to obtain stamps with replication of a hexagonal structure with elevated tips at initial interstices between the spheres. Aspect ratios of stamp features were optimized by adjusting the PDMS viscosity, by hydrophilisation of the substrate surface and by interlinking the spheres. We show a novel approach for tactile sensing with a transistor-based capacitive pressure sensor with promising characteristics for creation of an electronic skin.

O 60: Solid-liquid interfaces: Structure, Spectroscopy II

Time: Wednesday 10:30–11:45 Location: MA 144

O 60.1 Wed 10:30 MA 144

Adlayer formation of water and (co-)adsorbed CO on Ru(0001) and Pt$_{n\,\mathrm{ML}}$/Ru(0001) – A low temperature STM model study — •Martin Schilling, Sylvain Brimaud, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm

Understanding the processes occurring at the electrode | electrolyte interface is of fundamental interest to understand the electrochemical/-catalytic processes on a catalyst surface in an aqueous environment. The adsorption of water on monometallic single crystal surfaces can be considered as model system for the solid | electrolyte interface, and accordingly this has been studied intensely, including STM studies [1,2]. Here it is important to note, that for water adsorption adsorbate–adsorbate interactions play a pronounced, if not dominant role for the structure formation process. Here we report results of a low temperature STM study, where we investigated the adlayer formation of (co-)adsorbed water and CO on Pt$_{n\,\mathrm{ML}}$/Ru(0001) [3,4] and Ru(0001) surfaces under UHV conditions. We discuss first the observed structures, and the role of adsorbate–metal and adsorbate–adsorbate interactions. Next, we propose a kinetic model describing the adlayer formation, and finally we discuss the role of competing of different adsorbed species (H_2O, OH, CO, H) in the structure formation process. [1] J. Carrasco, A. Hodgson, A. Michaelides, *Nat.Mater.* **11** (2012) 667; [2] H.J. Yang, T. Minato, M. Kawai, Y. Kim, *J.Phys.Chem.C.* **117** (2013) 16429; [3] M. Schilling, S. Brimaud, R.J. Behm, *PCCP.* **19** (2017) 22434; [4] M. Schilling, S. Brimaud, R.J. Behm, *Surf.Sci.*, in press (2017).

O 60.2 Wed 10:45 MA 144

The Ionic Liquid|Graphite and Lithiated Graphite Interface - A Model Study for the Solid|Electrolyte Interphase in Li-ion Batteries — •Florian Buchner[1,2], Jihyun Kim[2], Katrin Forster-Tonigold[1], Isabella Weber[2], Johannes Schnaidt[1], Joachim Bansmann[2], Axel Gross[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

Here we report results of a UHV study on the interaction of an Ionic Liquid (IL) with graphite(0001) as a model study for the solid|electrolyte interphase (SEI) in Li-ion batteries. The interaction of mono- and multilayers of the battery-relevant IL 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide [BMP][TFSI] with pristine/lithiated graphite was investigated, employing X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS) and dispersion corrected density functional calculations (DFT-D). The measurements reveal that intact ion pairs adsorb on graphite, while deposition on lithiated graphite at 300 K (>230 K) leads to instantaneous deintercalation of Li^+. In general, contact of the IL with Li, either after deintercalation from lithiated graphite or after deposition from the vacuum side, results in the decomposition of the IL adlayer (Li_3N, Li_2S, etc.). The decomposition is different for multilayers. We will also compare the observed products with that in the electrochemical SEI in [Li][TFSI]/[BMP][TFSI].

O 60.3 Wed 11:00 MA 144

Potential-dependent distance-tunneling-current spectroscopy at the interface of gold(111) in an ionic liquid — •Marcel Lang, Stefan Herzog, Jeannete Lindner, and Rolf Schuster — Karlsruher Institute of Technologie, Karlsruhe, Germany

The behavior of ionic liquids at charged surfaces is fundamentally different from diluted electrolytes. For example ionic liquids form different multi-layered structures depending on the polarization of the gold electrode.

We investigated the interface [BMP][TFSA] on gold(111) using an STM under inertgas atmosphere operating at room temperature. We could observe two distincly different behaviours depending on the polarisation of the gold electrode. At potentials positive of -0.5 V vs Pt the barrier height steadily increases with distance. At potentials below -0.9 V vs Pt the barrier height shows local maxima and minima. The features in the measurements below -0.9 V vs Pt can be attributed to the structure of the first layer of the liquid.

O 60.4 Wed 11:15 MA 144

Time-resolved Electrochemical Surface Plasmon Resonance (SPR) Studies of the Aggregation of Surfactant Molecules at a Solid- liquid Interface — •Karin Schlag, Christian Kühn, Detlef Nattland, and Rolf Schuster — Karlsruhe Institute of Technology, Karlsruhe, Germany

The potential induced adsorption and phase transitions of dodecyl sulfate molecules on Au(111) have been studied with time-resolved surface plasmon resonance spectroscopy (a full plasmon profile per millisecond). Plasmons are excited at a 50 nm thin gold film working electrode using the Kretschmann configuration for attenuated total reflection. Position and shape of the curve are highly sensitive to the dielectric properties at the interface. Thus, changes of the coverage by fractions of a monolayer or variations of the thickness of an adsorbed layer can be detected. A multilayer model is used to interpret the plasmon profiles in which each layer is characterized by its thickness and its complex refractive index. While cycling through the phase transition from a hemicylindrical to a compact phase of the sodium dodecyl sulfate (SDS) system we obtained a shift to higher resonance angles with increasing potential. On the reverse direction we observe a hysteresis in the shift of the resonance angle. This finding is in line with potential pulse experiments, which imply a nucleation and growth process along this first order phase transition on a timescale of several 100 milliseconds.

O 60.5 Wed 11:30 MA 144

Hydration of Concrete: The first steps — •Peter Thissen, Nicolas Giraudo, Carsten Natzeck, and Christof Wöll — Karlsruher Institut für Technologie (KIT), Institut für Funktionelle Grenzflächen (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Concrete is the most important construction material used by mankind and, at the same time, one of the most complex substances known in materials science. Since this mineral compound is highly porous, a better understanding of its surface chemistry, and in particular the reaction with water, is urgently required to understand and avoid corrosion of infrastructure. We have gained insight into proton transfer from concrete upon contact with water by applying the so-called Surface Science approach to a well-defined mineral, Wollastonite. Data from infrared spectroscopy reveal that exposure of this Calcium-Silicate (CS) substrate to water leads to dissociation and the formation of OH-species. This proton transfer is a chemical reactions of key importance, since on the one hand it triggers the conversion of cement into concrete (a CSH phase), but on the other hand also governs the corrosion of concrete. Interestingly, we find that no proton transfer takes place when the same surface is exposed to methanol. In order to understand this unexpected differences, the analysis of the spectroscopic data obtained was aided by a detailed, first-principles computational study employing density functional theory (DFT). The combined experimental and theoretical effort allows deriving a consistent picture of proton transfer reactions occurring on CS and CSH phases.

O 61: Focus Session: Nanoscale Insights into Interfacial Electrochemistry I

Time: Wednesday 10:30–13:00 Location: HE 101

Invited Talk O 61.1 Wed 10:30 HE 101

Bias-dependent local structure of water molecules at a metallic interface — •Maria Victoria Fernandez-Serra — Physics and Astronomy department, Stony Brook University, Stony Brook NY 11794, USA

Understanding the local structure of water at the interfaces of metallic electrodes is a key issue in aqueous-based electrochemistry. Nevertheless a realistic simulation of such a setup is challenging, particularly when the electrodes are maintained at different potentials. To correctly compute the effect of an external bias potential applied to truly semi-infinite surfaces, we have combined Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) methods. This framework allows for the out-of-equilibrium calculation of forces and dynamics, and directly correlates to the chemical potential of the electrodes, which is introduced experimentally. I will review how the structure and work function of solvated Pd and Au electrodes depends on the nature of the water/metal interactions and relate this to the nature of the electrode and its surface charge.

Invited Talk O 61.2 Wed 11:00 HE 101

Optical imaging of surface chemistry and dynamics in confinement — •Sylvie Roke — 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

Electrochemical processes, chemical surface reactions and transformations at interfaces depend strongly on the local electrostatic environment as well as on nanoscale structures. In addition, structural heterogeneities, confinement, and flow critically influence surface chemical processes. Here, we image the interfacial structure and dynamics of water in a microscopically confined geometry in three dimensions and on millisecond time scales with a 3D structurally illuminated wide-field second harmonic microscope. Image contrast reports on the orientational order of interfacial water, induced by charge-dipole interactions between water molecules and surface charges. The images are converted into surface potential maps. Spatially resolved surface acid dissociation constant pKa,s values are determined for the silica deprotonation reaction by following pH induced chemical changes on the curved and confined surfaces of a glass micro-capillary immersed in aqueous solutions. These values ranged from 2.3 to 10.7 along the wall of a single capillary, because of surface heterogeneities. Water molecules that rotate along an oscillating external electric field were also imaged.

O 61.3 Wed 11:30 HE 101

Molecular dynamics study of the Mg(0001)/H_2O interface in an ab initio electrochemical cell — •Sudarsan Surendralal[1], Mira Todorova[1], Michael W. Finnis[2], and Jörg Neugebauer[1] — [1]Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH., Düsseldorf, Germany — [2]Department of Materials, Imperial College London, United Kingdom

Ab-initio modelling using density functional theory (DFT) provides important insight into the understanding of reactions at electrochemical interfaces. However, there is no commonly used method to tune the electrode potential in these simulations due to constraints imposed by the periodic boundary conditions common to many DFT codes. This is a major challenge for computational electrochemistry since it hampers observation of reactions under conditions of an applied potential. Utilizing semiconductor concepts, we have designed an approach to realize a potentiostat in standard periodic boundary DFT codes. Our approach allows the control of the electrode potential of the system by controlling the magnitude of charge transfer between two electrodes. Using this method, we study the Mg(0001)/H_2O interface under anodic polarisation conditions. The high corrosion rate under these conditions is a severe technological challenge and has thus been extensively studied. The atomistic mechanisms, however, could so far not be identified. Using the new approach, we are able to observe dissociation events, proton transfer as well as H_2 evolution and to identify a novel and hitherto not considered reaction mechanism.

O 61.4 Wed 11:45 HE 101

Influence of near surface defects of GaAs on the electrolyte structure in KOH solutions — •Alrik Stegmaier and Hans Hofsäss — 2. Physikalisches Institut, Georg-August Universität Göttingen

The electrolyte-semiconductor interface is a very active area of research. While the electrolyte structure at ideal, defect-free semiconductor surfaces is relatively well understood, the influence of surface near defects, applied potential differences and strong electrolytes, as found in many applications, is much more difficult to understand.

Here we present our latest results of our investigation of the structure of the electrolyte for defects near the <100>-GaAs - KOH/water interface at large pH values. For this classical and ab initio molecular dynamics simulations are combined with continuum models and impedance measurements for proton irradiated GaAs.

Invited Talk O 61.5 Wed 12:00 HE 101

Charge Transfer at the Single Molecule Level with Metal and Semiconductor Electrodes — •Richard Nichols[1], Andrea Vezzoli[1], Richard Brooke[2], Nicolò Ferri[1], Simon Higgins[1], and Walther Schwarzacher[2] — [1]Department of Chemistry, University of Liverpool, L69 7ZD, UK — [2]University of Bristol, Bristol BS8 1TL, UK

We have exploited STM based methods for making single molecule measurements on a wide variety of molecular targets from short molecular bridges to redox active organometallic molecular wires. Such measurements have been made as 2-terminal determinations and also under electrochemical control with electrolytes including ionic liquids. Recently we have extended such measurements to semiconductor electrodes. We have shown that it is possible to make measurements of single molecules connected at one end to gallium arsenide and at the other end to a gold STM tip. Using this methodology we can record current-voltage response of semiconductor-molecule-metal devices and measure the electrical conductance of single molecules in such junctions. As well as showing that it is possible to form single molecule devices contacted to the semiconductor gallium arsenide we have also recently demonstrated that such single molecule devices show a strong photocurrent response. The photo-current response in these junctions can be controlled through the choice of the semiconductor doping density, the molecular bridge and also the light intensity and wavelength. To conclude potential future applications in single-molecule semiconductor (photo-) electrochemistry will be discussed.

O 61.6 Wed 12:30 HE 101

***In-operando* Vibrational Spectroscopies in Electrochemical Environment from First-principles** — •Francesco Nattino[1], Oliviero Andreussi[1,2], and Nicola Marzari[1] — [1]Theory and Simulations of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Station 12, CH-1015 Lausanne, Switzerland. — [2]Institute of Computational Science, Università della Svizzera Italiana, Via Giuseppe Buffi 13, CH-6904 Lugano, Switzerland.

Electrocatalysis is expected to play a key role in the development of a clean energy cycle, from energy harvesting to transformation and storage. Spectroscopic techniques able to work under potential control can extremely contribute to design novel catalyst materials by providing insight on the mechanism of target electrochemical reactions. In this context, theory has the task to decipher the precious information that *in-operando* experimental techniques are able to provide.

We present here first-principles calculations on key reaction intermediates of two electrochemical processes: the oxidation of a gold single crystal surface and the carbon dioxide reduction on copper metal electrodes. Vibrational adsorbate frequencies are computed in a realistic electrochemical environment, exploiting an accurate implicit solvation model to mimic the electrolyte solutions. Our results complement very recent surface enhanced Raman spectroscopy (SERS) experiments and surface enhanced IR absorption (SEIRA) measurements, contributing to shed light on the reaction mechanism of the two electrocatalytical processes considered.

O 61.7 Wed 12:45 HE 101

Quasi-atomistic insight into Au oxide reduction under realistic working conditions — •Jonas H. K. Pfisterer, Ulmas E. Zhumaev, and Katrin F. Domke — Max Planck Institute for Polymer Research, Mainz, Germany

The rational design of improved electrochemical devices, e.g. fuel cells, depends on the atomistic understanding of the underlying reaction processes under realistic working conditions. The ability of tuning the Fermi level and employing highly sensitive molecular detection methods can provide valuable insights into molecular adsorption/desorption on the surface. Here, we investigate the reduction of AuOx surfaces in contact with an electrolyte by in-situ surface-enhanced Raman scattering (EC-SERS). We have performed potential-jump experiments in which we stepwise vary the applied potential to induce either AuOx formation or Au surface recovery. As a function of potential, we observe a splitting of the AuOx/(AuOH) peak at 585 cm^{-1} into two peaks that are assigned to AuOx and AuOH based on H/D exchange experiments. Further, the AuOH peak exhibits Raman intensity oscillations with time that can possibly be ascribed to subsurface OH moving to the surface. Accompanying Raman peaks at 240 and 1200 cm^{-1}, complemented with in-situ IR absorption experiments, indicate that the adsorption of $\mathrm{SO_4}^{2-}$ starts only after initial AuOx reduction.

Our potential-jump experiments on AuOx surfaces reinforce the role of OH species for the reduction process even in acidic media and represent an interesting approach to gain quasi-atomistic insights into surface reactions under realistic working conditions.

O 62: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 10:30–13:00 Location: HL 001

Invited Talk O 62.1 Wed 10:30 HL 001

Correlating electrons via adiabatic connection approach: a general formalism, approximations, and applications — •Katarzyna Pernal — Institute of Physics, Lodz University of Technology, Poland

Electronic systems are usually described by assuming a model Hamiltonian, which only partially recovers electron correlation effects. To assure a quantitative description one faces a problem of recovering the missing part of the correlation. Over years different methods have been developed, most of them originating from the perturbation theory.

In my talk I will present another, fairly general, approach based on the adiabatic connection formalism. The idea itself is not novel although it has not been considered as a way of adding electron correlation for multireference models. Until recently it has not been realized that by combining the adiabatic connection (AC) with the extended random phase approximation one obtains a general tool capable of accounting for dynamical electron correlation for a broad class of multireference wavefunctions, applicable even to systems including strongly correlated electrons. It will be shown that the AC-based approximation yields excellent results when applied to multireference models, exceeding in accuracy second-order perturbation-theory-based methods.

O 62.2 Wed 11:00 HL 001

Density functional theory of electron transfer beyond the Born-Oppenheimer approximation: case study of LiF — •Chen Li[1], Ryan Requist[1], and Eberhard. K. U. Gross[1,2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel

We demonstrate that beyond Born-Oppenheimer (BO) effects can be accurately and seamlessly incorporated within a density functional framework. In alkali halides like LiF, there is an abrupt change in the ground state electronic distribution due to an electron transfer at a critical bond length $R = R_c$. We find that nonadiabatic electron-nuclear coupling produces a sizable elongation of the critical R_c by 0.5 Bohr, an effect which is very accurately captured by a simple and rigorously-derived nuclear mass-dependent correction to the exchange-correlation potential in density functional theory. Since this nonadiabatic term depends on gradients of the nuclear wave function and conditional electronic density, $\nabla_R \chi(R)$ and $\nabla_R n(r, R)$, it couples the Kohn-Sham equations at neighboring R points. Motivated by an observed localization of nonadiabatic effects in nuclear configuration space, we propose an approximation that reduces the search for nonadiabatic density functionals to the search for a single function. This work is a step towards bringing density functional theory beyond the limitations of the BO approximation.

O 62.3 Wed 11:15 HL 001

Ground-State Quantum-Electrodynamical Density-Functional Theory — •Michael Ruggenthaler — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

In this talk I present a density-functional reformulation of correlated matter-photon problems subject to general external electromagnetic fields and charge currents [1]. I first show that for static minimally-coupled matter-photon systems an external electromagnetic field is equivalent to an external charge current. I employ this to show that scalar external potentials and transversal external charge currents are in a one-to-one correspondence to the expectation values of the charge density and the vector-potential of the correlated matter-photon ground state. This allows to establish a Maxwell-Kohn-Sham approach, where in conjunction with the usual single-particle Kohn-Sham equations a classical Maxwell equation has to be solved in order to capture the correlation induced by the transversal photon field. In the magnetic mean-field limit this reduces to a current-density-functional theory that does not suffer from non-uniqueness problems and if furthermore the magnetic field is zero recovers standard density-functional theory.

[1] ”Ground-State Quantum-Electrodynamical Density-Functional Theory”, M. Ruggenthaler, arXiv:1509.01417 (2017).

O 62.4 Wed 11:30 HL 001

Design of auxiliary systems for observables: the dynamic structure factor and the electron addition and removal spectra — Marco Vanzini, Martin Panholzer, Lucia Reining, and •Matteo Gatti — LSI, CNRS, Ecole Polytechnique, Palaiseau, France

Density functional theory tells us that the external potential, and therefore all observables, are functionals of the ground state density. The exact functionals, however, are not known, and one has to find approximations. To obtain the density, Kohn and Sham have proposed the idea to use an “auxiliary system”. Much research effort goes into finding better and better Kohn Sham potentials for the density and the total ground state energy. In order to access also observables other than the density, we have proposed to generalize the Kohn-Sham idea of an auxiliary system [1], and to design a “connector” that allows us to profit from calculations done in a model system [2,3]. We have recently shown that this is a successful strategy for the dynamic structure factor [2] and for the one-body spectral function of simple metals, semiconductors and insulators [3]. [1] M. Gatti, V. Olevano, L. Reining, and I. V. Tokatly, Phys. Rev. Lett. 99, 057401 (2007) [2] M. Panholzer, M. Gatti, and L. Reining, arXiv:1708.02992 [3] M. Vanzini, L. Reining, and M. Gatti, arXiv:1708.02450

O 62.5 Wed 11:45 HL 001

Exact exchange energy of the ferromagnetic electron gas with dipolar interactions — •Camilla Pellegrini, Tristan Mueller, Kay Dewhurst, Sangeeta Sharma, and Eberhard K. U. Gross — Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We propose a density functional treatment of the magnetic dipole-dipole interaction as a spin-spin correction to the Coulomb force in the Breit-Pauli Hamiltonian. Within this microscopic approach, the Hartree-like term for the dipolar coupling corresponds to the classical magnetostatic energy currently implemented in micromagnetic calculations. In addition, we have derived quantum corrections by evaluating analytically the exact exchange energy (Fock term) for the homogeneous electron gas, within the linear response to a noncollinear magnetic field. We expect our functional to open the path towards a full ab initio description of inhomogeneous magnetic structures at the nanoscale, with applications to domain-wall operated spintronic devices.

O 62.6 Wed 12:00 HL 001

Precise total-energy calculations at a significantly reduced cost — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In density-functional calculations, the total-energy functional is stationary with respect to the density, the Kohn-Sham orbitals and the Kohn-Sham effective potential. This means that approximations for these quantities only lead to total-energy errors of second order provided that the total-energy functional is evaluated accurately without further uncontrolled approximations.

Unfortunately, usually the Kohn-Sham orbitals and thus the kinetic part of the total energy are evaluated by using a projection of the potential into a finite subspace of basis functions. This approximation damages the stationarity of the total energy as a functional of the potential.

A technique will be discussed which can relieve this deficiency so that a considerably smaller subspace of basis functions can be used for a precise evaluation of the kinetic part of the total energy. The advantage will be illustrated for the particular example of angular projection potentials as they are used in the full-potential Korringa-Kohn-Rostoker Green function method.

O 62.7 Wed 12:15 HL 001

Approach to Orbital-free DFT with Englert-Schwinger model — •Jouko Lehtomäki and Olga Lopez-Acevedo — COMP Centre of Excellence, Department of Applied Physics, Aalto University, Finland

We briefly present the Englert and Schwinger (ES) model in comparison with other approaches to orbital-free DFT. Essential failure of many kinetic energy density functionals is that they can not describe the most tightly bound core electrons in a satisfactory manner. Englert-Schwinger model allows treating these problematic electrons with more accurate single-particle wavefunctions while still obtaining the self-consistent orbital-free solution to the electronic problem.

Specifically, we detail how the ES model compares to the more known Thomas-Fermi-Dirac-Weizsäcker model self-consistently in atoms. We look at the total energy and few geometric properties. We show qualitative improvement in Pauli potential, which shows unphysical singularities near nucleus when the most tightly bound electrons are not treated correctly. We present how augmentation of the model with Kohn-Sham orbitals allows us to explore all-electron solution to the OFDFT problem and how this paves way for an orbital-free DFT method which does not need pseudopotentials.

O 62.8 Wed 12:30 HL 001

The Kerker Preconditioner for FLAPW Methods with Charge Density Mixing — •Miriam Hinzen, Edoardo Di Napoli, Daniel Wortmann, and Stefan Blügel — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In metallic systems of larger size the self-consistent field convergence of electronic structure calculations is often slowed down substantially due to charge sloshing: close to the Fermi level, little change in energy can cause large fluctuations in charge density. Mathematically speaking, the problem is ill-conditioned. For plane-wave methods the Kerker preconditioner effectively solved this problem, but for many other electronic structure methods, in particular all-electron methods as the FLAPW or KKR methods, a real-space formulation would be needed. We developed a formulation of the Kerker preconditioner for FLAPW methods with charge density mixing, implemented in `FLEUR` [1]. Numerical experiments show an enormous reduction of the number of iterations needed for convergence; even more importantly, the SCF convergence has become independent of the system size.
[1] www.flapw.de

O 62.9 Wed 12:45 HL 001

Effect of spin on the generalized Pauli constraints in Reduced Density Matrix Functional Theory — •Nicole Helbig[1], Iris Theophilou[2], and Nektarios N. Lathiotakis[3] — [1]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, GR-11635 Athens, Greece

Reduced Density Matrix Functional Theory is a method that relies on the 1-1 correspondence between the many-body ground-state wave function and the first order reduced density matrix (1RDM) and uses the latter as its fundamental variable. Enforcing the generalized Pauli constraints during the energy minimization ensures that the 1RDM corresponds to a fermionic pure state. We demonstrate that these constraints are modified for open-shell systems if the spin degrees of freedom are taken into account. From the generalized Pauli constraints we also derive properties of the exact occupation numbers and natural orbitals which ensure that the 1RDM corresponds to an eigenstate of the total spin.

O 63: Plasmonics and nanooptics: Applications and other aspects I

Time: Wednesday 12:00–13:00 Location: MA 041

O 63.1 Wed 12:00 MA 041

Heat transfer along a chain of nanoparticles — •Christoph Kathmann[1], Philippe Ben-Abdallah[2], and Svend-Age Biehs[1] — [1]Institut für Physik, Oldenburg University, Germany — [2]CNRS, Laboratoire Charles Fabry, Palaiseau, France

In the near field, the radiative heat flux transferred between two bodies can overcome the predictions made by Planck's law by several orders of magnitude due to the contribution of evanescent modes. We consider a chain of SiC nanoparticles with the distance between the particles being small enough to allow the coupled surface phonon polaritons to propagate along the chain. The resulting heat transfer is calculated numerically exact using fluctuating electrodynamics and compared to results from a ballistic and a diffusive approach based on Landauer and Boltzmann equation.

O 63.2 Wed 12:15 MA 041

Ultrafast point-projection electron microscopy with a time-of-flight delay-line detector — •Germann Hergert[1], Andreas Wöste[1], Jan Vogelsang[1], Dong Wang[2], Petra Gross[1], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany — [2]Institut für Werkstofftechnik, TU Ilmenau, 98693 Ilmenau, Germany

Observing electrons move on their natural few-fs-time and nm-spatial regime requires ultrahigh resolution. In laser-triggered ultrafast electron microscopes the temporal resolution typically is limited to around 100fs by the mesoscopic propagation distance of the probing electron pulse to the sample, which leads to pulse broadening due to dispersion.

One way to overcome this broadening is to reduce the distance between emitter and sample. An already known solution to this is adiabatic nanofocusing of surface plasmon polaritons along the shaft of a sharp metallic taper. This prevents direct illumination of a sample and allows minimal distances to the emitter. Implementing this method into an ultrafast point-projection electron microscope (UPEM) allows imaging with unprecedented spatio-temporal resolution. We equip the system with a time-of-flight delay-line detector to gain additional information about the electron energies for studying the interaction between electrons and localized electric fields, e.g. around nanostructures.

Here, we present such an UPEM setup with high spatio-temporal resolution. We show first results, where we photoemit electrons from nanometer-sized plasmonic antennas with femtosecond laser pulses and observe their motion with 20-nm spatial and 25-fs temporal resolution.

O 63.3 Wed 12:30 MA 041

Directional emission from dielectric antennas: A parameter study — •Till Leuteritz and Stefan Linden — Physikalisches Institut, Universität Bonn, D-53115

Metal nanostructures can be used as optical antennas to shape the far field emission pattern of quantum dots to achieve directional emission with large front-to-back ratios. In order to get a broadband emission and to have low losses, dielectric materials are a great candidate for these structures. Following this approach, M. Peter et al demonstrated recently a dielectric leaky-wave antenna made from Hafniumdioxide (HfO2) with a front-to-back ratio of around 12.5 dB [1].

In this presentation, we report on a systematic study of the dependence of the emission properties of dielectric leaky wave antenna on the geometrical parameters. The antennas consist of only two simple dielectric building blocks, a director and a reflector, whose length, height and width is parametrically changed. Quantum dots placed in between reflector and director serve as internal light source.

We find that by varying the width, the director changes from a leaky waveguide to a transversal single mode guided waveguide to a transversal multimode guided waveguide. Moreover, we observe that short leaky waveguides exhibit a bright emission peak at small angles that shifts to larger angles with increasing length. A similar behavior is also found for the transversal single mode guided waveguides.

[1] Directional Emission from Dielectric Leaky-Wave Nanoantennas; Manuel Peter et al.; Nano Letters 2017 17 (7), 4178-4183; DOI: 10.1021/acs.nanolett.7b00966

O 63.4 Wed 12:45 MA 041

Robustness of a nontrivial edge mode against periodic perturbations of a topological defect in a plasmonic waveguide array. — •Zlata Cherpakova and Stefan Linden — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

The Su-Schrieffer-Heeger (SSH) model describing a chain of identical lattice sites with alternating strong and weak bonds exhibits nontrivial edge states which are known to be robust against static deformations. Of special interest is to probe the robustness of these states against temporal perturbations. Here, we investigated the influence of periodic fluctuations on the topological edge mode in the plasmonic analogue of the SSH model. The plasmonic structures were fabricated by making use of negative-tone gray-scale electron beam lithography. Based on the quantum-optical analogy, the SSH chain was realized in an array of identical plasmonic waveguides with alternating long and short center-to-center distances. The temporal perturbations of the topological defect were implemented by periodically bending the central waveguide at the interface between two SSH domains. Surface plasmon polaritons were excited by shining a highly focused laser beam on the grating, deposited on top of the central waveguide. The spatial evolution of the SPP field intensity was monitored by real- and Fourier space leakage radiation microscopy. In our experiments as well as in numerical calculations we observe that if the frequency of these periodic perturbations was in the range which allows to overcome the bandgap, the edge mode couples to the bulk modes and becomes delocalized.

O 64: Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures IV

Organizers: Sabine Maier, FAU Erlangen-Nürnberg; Meike Stöhr, University of Groningen

(Synopsis provided with part I of this session)

Time: Wednesday 15:00–18:15 Location: MA 004

O 64.1 Wed 15:00 MA 004

Crystallization of a Two-Dimensional Hydrogen-Bonded Molecular Assembly: Evolution of the Local Structure Resolved by Atomic Force Microscopy — •Laerte L. Patera[1], Xunshan Liu[2], Nico Mosso[3], Silvio Decurtins[2], Shi-Xia Liu[2], and Jascha Repp[1] — [1]University of Regensburg, Regensburg, Germany — [2]University of Bern, Bern, Switzerland — [3]IBM Research-Zurich, Rüschlikon, Switzerland

Noncontact Atomic Force Microscopy (nc-AFM) provides detailed insights into the structure of surface-supported molecular self-assemblies, overcoming restrictions given by scanning tunneling microscopy (STM). Here we resolved the structures of the aromatic N-heterocyclic hexaaza-triphenylene (HAT) molecular synthon with sub-Å resolution by means of nc-AFM, both in the kinetically trapped amorphous state and in the thermo-dynamically stable crystalline phase. These results reveal how the crystallization governs the length scale of the network order for non-flexible molecular species without affecting the local bonding schemes. The capability of nc-AFM to accurately resolve structural relaxations will be highly relevant for the characterization of vitreous two-dimensional supramolecular materials.

O 64.2 Wed 15:15 MA 004

Assigning the absolute configuration of chiral aliphatic compounds by direct visual inspection of individual molecules — Daniel Ebeling[1], Marina Sekutor[2], Marvin Stiefermann[1], Jalmar Tschakert[1], Jeremy Dahl[3], Robert Carlson[3], Peter Schreiner[2], and •Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig University Giessen, Germany — [2]Institute of Organic Chemistry, Justus-Liebig University Giessen, Germany — [3]cStanford Institute for Materials and Energy Sciences, Stanford, USA

Deciphering the absolute configuration of a single molecule by direct visual inspection is the next step in direct compound identification, with far-reaching implications for medicinal chemistry, pharmacology, and natural product synthesis. Here we demonstrate the feasibility of this approach utilizing low temperature atomic force microscopy (AFM) with a CO-functionalized tip to determine the absolute configuration and orientation of single adsorbed [123]tetramantane molecule, the smallest chiral diamondoid. We differentiate between single enantiomers on a Cu(111) surface by direct visual inspection with atomic precision, and furthermore identify molecular dimers and small molecular clusters. The experimental results were also confirmed by a computational study that additionally allowed quantification of the corresponding intermolecular interactions. The unique toolset of absolute configuration determination combined with AFM tip manipulation now opens the route for unprecedented molecular nucleation studies, including chirality driven assembly or reaction mechanisms.

O 64.3 Wed 15:30 MA 004

Surface induced asymmetric activation of 4,4”-Diamino-p-terphenyl on Cu(111): symmetry breakdown by lattice mismatch — Qigang Zhong[1], •Daniel Ebeling[2], Jalmar Tschakert[2], Yixuan Gao[3], Deliang Bao[3], Shixuan Du[3], Lifeng Chi[1], and Andre Schirmeisen[2] — [1]Institute of Functional Nano & Soft Materials, Soochow University, Suzhou, China — [2]Institute of Applied Physics, Justus-Liebig University, Giessen, Germany — [3]Institute of Physics, Chinese Academy of Sciences, Beijing, China

We demonstrate that asymmetric activation of the mirror symmetric molecule 4,4”-Diamino-p-terphenyl (DATP) is possible on a metal surface. Our low temperature atomic force microscopy images, using CO-tip functionalization, show that on Cu(111) the DATP the adsorption geometry becomes asymmetric for certain orientations, while on Au(111) the symmetry is fully retained. This symmetry breaking on Cu(111) is caused by a lattice mismatch between the molecule and the metal surface, corroborated by interactions with the subsurface atomic layer. The asymmetric DATP molecules show non-stationary behavior under the influence of the scanning tip, which leads to a bi-level telegraph noise, here serving as a fingerprint of the surface induced asymmetry. Dispersion corrected DFT-D2 computations confirm the precise topology, the dynamics, and the energy barriers of the observed asymmetric adsorption geometries. Finally, we exploit the asymmetric activation of DATP for side-preferential attachment of 2-triphenylenecarbaldehyde (TPCA). Our findings provide a new route for surface induced asymmetric activation of a symmetric compound.

O 64.4 Wed 15:45 MA 004

Interaction of molecules with doped graphene via noncovalent interactions — •Bruno de la Torre[1,2], Martin Svec[1,2], Rabindranath Lo[3], Pavel Jelinek[1,2], Radek Zboril[2], and Pavel Hobza[2,3] — [1]Regional Centre of Advanced Technologies and Materials, Palacký University, Olomouc, Czech Republic. — [2]Institute of Physics of the CAS, Prague, Czech Republic. — [3]Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic.

Chemical doping of graphene is an efficient way of tuning its intrinsic properties. In particular, implantation of a single-atom dopant [1,2] modifies graphene local electronic structure and consequently its chemical activity [3]. Understanding the interaction of molecules with individual dopants in graphene is of immense importance for development of graphene-based devices. We study the interaction of iron(II) phthalocyanine (FePc) with both pristine and N-doped graphene by means of cryogenic STM+AFM. While on pristine graphene the FePc forms regularly ordered self-assemblies, the presence of nitrogen dopants anchors FePc non-covalently, preventing their long-range ordering (see Fig.1). By STS and manipulation with the molecules we investigate how the proximity of the N-dopant affects the electronic states of a FePC molecule. The AFM high-resolution imaging with a CO-tip reveals a substantial charge redistribution within the molecule.

[1] M. Telychko et al. ACS Nano 8 (7), 7318 (2014), [2] A. Martin-Recio et al. Nanoscale 8, 17686 (2016) [3] M. Telychko et al. ACS Nano 9 (9), 9180 (2015)

O 64.5 Wed 16:00 MA 004

Resolving molecular products of surface induced chemical reactions of 9-Azidophenanthrene — •Aleš Cahlík[1], John Hellerstedt[1], Pingo Mutombo[1], Oleksander Stetsovych[1], Ivo Starý[2], Irena Stará[2], Martin Švec[1], and Pavel Jelínek[1] — [1]Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic — [2]Institute of Chemistry and Biochemistry, Czech Academy of Sciences, Praha, Czech Republic

The preparation of suitable systems for controllable, light-driven molecular switches presently remains an appealing experimental challenge. Recently, azo-compounds have proven to be an auspicious choice for such purpose. We report the on-surface synthesis and identification of azo-phenanthrene isomers, a prospective molecular switch, using azide-based 9-Azidophenanthrene (APT) as a molecular precursor. Due to the high reactivity of APT, a broad variety of reaction pathways exist which results in an extensive mixture of products. Such chemical diversity is hard to grasp by means of a conventional chemical analysis tools owing to the subtle structural differences with nearly identical bond environments. In our experiment, we went beyond the limits of these techniques by employing non-contact atomic force microscopy to achieve submolecular resolution of the product species. We speculate that the precursor decomposes into highly reactive nitrene species, that subsequently form a diverse mixture of products. By close comparison with theoretical calculations we are able to distinguish between covalently (N=N) bonded azo-phenanthrene isomers and other non-covalently bonded molecular structures.

O 64.6 Wed 16:15 MA 004

On-surface synthesis of nitrogen-doped 5-7-membered nanographenes — •Frank Eisenhut[1,2], Dmitry Skidin[1,2], Justus Krüger[1,2], Marcus Richter[1,3], Reinhard Berger[1,3], Xinliang Feng[1,3], Francesca Moresco[1,2], and Gianaurelio Cuniberti[1,2,4] — [1]Center for Advancing Electronics Dresden (cfaed), TU Dresden, 01062 Dresden, Germany — [2]Institute for Materials Science, TU Dresden, 01069 Dresden, Germany — [3]Institute for Molecular Functional Materials, TU Dresden, 01062 Dresden, Germany — [4]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01069 Dresden, Germany

We present the on-surface synthesis of five- and seven-membered nitrogen-doped "defective" nanographene molecules by thermally induced cyclodehydrogenation of a nitrogen-containing polycyclic hydrocarbon on the Au(111) surface. The reaction is investigated by scanning tunneling microscopy (STM) at low-temperature. After annealing, we observe mainly non-symmetric planar products. High-resolution STM images on single molecules show the formation of a five- and a seven-membered ring, while the planarity is obtained by the cleavage of one phenyl-group. In a few cases, we observe non-planar bowl-shaped molecules with an Azacorannulene core. This indicates the complete conversion of the precursor molecule into a nitrogen-doped nanographene with four odd-numbered rings. Using scanning tunneling spectroscopy, we investigate the electronic structure of all molecular species.

15 min. break

O 64.7 Wed 16:45 MA 004

The role of tip reactivity in intramolecular imaging of organic molecules in NC-AFM — •Adam Sweetman[1], Sam Jarvis[2], Philipp Rahe[3], and Philip Moriarty[1] — [1]School of Physics and Astronomy, University of Nottingham, U.K. — [2]School of Physics, University of Lancaster, UK — [3]Department of Physics, University of Osnabrück, Germany

Noncontact atomic force microscopy (NC-AFM) is now routinely capable of obtaining submolecular resolution, readily resolving the carbon backbone structure of planar organic molecules adsorbed on metal substrates. However, normally this resolution requires functionalisation of a metal tip by a carbon monoxide (CO) molecule or similar passivating group.

In this work, we show that the same resolution may also be obtained for molecules adsorbed on a reactive semiconducting substrate, and that surprisingly, this resolution is routinely obtained without the need for deliberate tip functionalization [1].

Counter to intuitive expectations, we find that many silicon terminated tips do not react strongly with the adsorbed organic molecules, and we find that only specific highly oriented clusters have sufficient reactivity to break open the existing carbon-carbon bonds [2]. Our results suggest a wide range of tips may be capable of producing intramolecular contrast for molecules adsorbed on semiconductor surfaces.

1. Sweetman, A. et al. Phys. Rev. B 94, 115440 (2016).
2. Sweetman, A. et al. Phys. Rev. B 90, 165425 (2014).

O 64.8 Wed 17:00 MA 004

Probing intermolecular interactions in a molecular layer via single-molecule manipulation — •Christian Wagner^{1,2}, Philipp Leinen^{1,2}, Alexander Diener^{1,2}, Ruslan Temirov^{1,2}, and F. Stefan Tautz^{1,2} — ^{1}Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — ^{2}Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology, Jülich, Germany

Adsorption of large organic molecules is often influenced by their functional groups which may simultaneously interact with the surface and neighboring molecules. Together with the mechanical flexibility of molecules this leads to a multidimensional, highly structured and typically rather shallow interaction potential landscape which can hardly be investigated by any other means than theoretical simulations. Here we show that non-contact atomic force microscopy (NC-AFM) facilitates single-molecule manipulation protocols which enable probing the potential energy surface in a molecular layer. We apply the manipulation to the archetypal model system PTCDA (perylene-3,4,9,10-tetracarboxylic dianhydride) on Ag(111) and study the influence of polar groups, specifically of weak hydrogen bonds on the intermolecular potential. Fitting a force-field model to our experimental data reveals how electrostatic interactions cause out-of-plane forces on partially charged atoms. Our results intuitively explain how such interactions can alter the vertical adsorption geometry of a molecule in a layer compared to an isolated molecule.

O 64.9 Wed 17:15 MA 004

Mechanical response while pulling a single poly-pyrene chain on gold — •Rémy Pawlak^{1}, Philipp D'Astolfo^{1}, Guilherme Vilenha^{2}, Tobias Meier^{1}, Thilo Glatzel^{1}, Shi-Xia Liu^{3}, Silvio Decurtin^{3}, Ruben Perez^{2}, and Ernst Meyer^{1} — ^{1}Physics Department,University of Basel, Switzerland — ^{2}Departamento de Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, Spain — ^{3}Department of Chemistry and Biochemistry, University of Berne, Switzerland

The intamolecular mechanics of a molecule govern its diffusion while sliding over a surface. Quantifying such aspect at the molecule level is however challenging and poorly observed so far [1-3]. Here, we synthesized long polypyrene chains linked by C-C bonds on Au(111) and proceed to their vertical and lateral manipulations with the apex of an atomic force microscope. Combined force measurements and numerical calculations show that periodic modulations in the force response arise from the detachment of single pyrene units from the surface as well as their sliding over the surface lattice potential. These periodicities show that the remaining pyrene on the surface "snake" during manipulations to adapt its commensurability with the surface lattice as well as reduce the mechanical stress induced by the lifted units. [1] Kawai et al. Proc. Natl. Acad. Sci. USA 2014, 111, 3968-3972. [2] Kawai et al. Science 2016, 351, 957-961. [3] Pawlak et al. ACS Nano 2016 10, 713-722

O 64.10 Wed 17:30 MA 004

Single molecule manipulation via inelastic electron tunneling — •Gitika Srivastava^{1}, Tibor Kudernac^{2}, Manfred Parschau^{1}, Peter Stacko^{3}, Bernard L. Feringa^{3}, and Karl-Heinz Ernst^{1,4} — ^{1}Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — ^{2}University of Twente, The Netherlands — ^{3}Univeristy of Groningen, The Netherlands — ^{4}University of Zürich, Switzerland

Maneuvering individual molecules over a clean and unmodified surface is challenging, yet possible using surface sensitive techniques like Scanning Tunneling Microscopy (STM). Electronic and vibrational excitation by means of inelastic electron tunneling from the tip of STM has been observed to have brought out subsequent dynamical processes on surfaces. We investigate the influence of inelastic electron tunneling on molecules with two functional unidirectional rotor units, comparable to the previously reported 4-wheeler as nano-car and have observed molecular motions like hopping and conformational changes. Results of single molecular dynamics of these molecules at low temperatures (6K) on Cu(111) surface are presented and discussed.

O 64.11 Wed 17:45 MA 004

Controlled dissociation of intramolecular bonds by STM manipulation — •Donato Civita^{1}, Stefan Hecht^{2}, and Leonhard Grill^{1} — ^{1}Department of Physical Chemistry, University of Graz, Austria — ^{2}Institute of Chemistry, Humboldt-Universität zu Berlin, Germany

Manipulation of molecules adsorbed at surfaces is very appealing to control and understand fundamental chemical processes. Chemical reactions can be triggered in single molecules by using the energy of the tunneling electrons in a scanning tunneling microscope (STM). Specifically, chemical bonds within molecules can be cleaved [1], the resulting fragments can be pulled across the surface by lateral manipulation with the STM tip and even new bonds can be formed [2].

In this work, we study the dissociation of single Br atoms from dibromoterfluorene (DBTF) molecules adsorbed on the Ag(111) surface. Experiments were done with a low temperature STM and applying voltage pulses where the Br substituents are located. By studying the current signal during the voltage pulse as well as imaging the single molecule before and after such a manipulation, we obtain insight into the process. After dissociation, single Br atoms and the remaining molecule are laterally dislocated over the surface, which reveals details about the interatomic interactions.

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

[2] S.-W. Hla, L. Bartels, G. Meyer, and K.-H. Rieder, Phys. Rev. Lett. 85, 2777 (2000)

O 64.12 Wed 18:00 MA 004

Reversible 2D phase transition driven by an electric field: visualization and control on the atomic scale — Ben Wortmann^{1}, Dennis van Voerden^{1}, •Paul Graf^{1}, Roberto Robles^{2}, Paula Abufager^{2}, Nicolás Lorente^{2}, Christian Bobisch^{1}, and Rolf Möller^{1} — ^{1}Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany — ^{2}ICN2 Catalan Institute of Nanoscience and Nanotechnology, CSIC and The Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain

We report on a reversible structural phase transition of a two dimensional system which can be locally induced by an external electric field. [1] By means of scanning tunneling microscopy (STM) we determined two coexisting structural configurations of a CO monolayer on Cu(111): an α-phase (7×7 superstructure) and a β-phase ($3\sqrt{3} \times 3\sqrt{3}$) R30°. The balance of the two phases can be shifted by the electric field of the STM tip, causing the domain boundaries to move, increasing the area of the favored phase controllable both in location and size. If the field is further enhanced new domains nucleate. The arrangement of the CO molecules on the Cu surface is observed in real time and real space with atomic resolution while the electric field driving the phase transition is easily varied over a broad range.Our new manipulation mode permits us to bridge the gap between spontaneous long-range ordering of phase transitions and man-made CO structures created by molecular manipulation of CO adlayers.

[1] B. Wortmann et al., Nano Letters **16** (1), 528-533 (2016)

O 65: Focus Session: Structure and Chemistry of Metal-Oxide Surfaces III

Time: Wednesday 15:00–16:45 Location: MA 005

O 65.1 Wed 15:00 MA 005

Density functional theory study of water and glycine adsorption at TiO2-TiN interfaces — •Julio Gutierrez Moreno and Michael Nolan — Tyndall National Institute, University College Cork

Titanium nitrite (TiN) is used in sensors as a conducting layer with good hardness and resistance to corrosion. TiN can spontaneously form a thin oxide layer when it is exposed to air, which could modify the properties of the coating and the impact on biofouling is not yet clear. Therefore, there is significant interest in studying the biofouling of oxidised TiN to find strategies to inhibit this process. In this work, we carried out Hubbard corrected density functional theory (DFT+U) simulations of the TiO2-TiN interface, as a model of the oxide layer on TiN. We investigate defects that can form during the oxide growth and are present after TiO2 formation such as Ti vacancies in TiN, O vacancies or the interdiffusion of O/N atoms within the interface. Our simulations show the formation of Ti3+ cations in the TiO2 that arise upon interface formation. We found that water adsorbs dissociatively on TiO2-TiN for low surface coverages while molecular adsorption is more stable are higher coverage. Glycine adsorption from gas phase is strong on the TiO2-TiN interface (E=-1.6 eV) compared to bare TiN (E=-0.4 eV). However the adherence of glycine is weaker on hydrated surfaces and also depends on the defects that might be present in the interface. The outcomes of these simulations give us a more comprehensive insight on the atomic level structure and the electronic properties of oxidised TiN surfaces and how this is related to biofouling.

O 65.2 Wed 15:15 MA 005

Influence of halic and carboxylic acids on the shape of TiO$_2$ nanoparticles — Kai Sellschopp[1], Wolfgang Heckel[1], Andreas Hensel[2], Clemens Schröter[2], Tobias Vossmeyer[2], Horst Weller[2], Stefan Müller[1], and •Gregor Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]Institute of Physical Chemistry, University of Hamburg

Titania (TiO$_2$) nanoparticles are used for many applications ranging from photo-catalysts to hybrid materials. The faceting and accordingly the shape of the nanoparticles determine the performance of the nanoparticles in these applications. Therefore, shape control during synthesis is essential. It is known that fluoric acid stabilizes the anatase (001) surface through a substitution of surface oxygen atoms. This leads to platelet shaped particles with a large percentage of reactive (001) facets. The influence of other halic and organic acids on the particle shape, however, is rarely studied. Here, we present our latest results on the adsorption and surface energies of all halic acids and some carboxylic acids on the major TiO$_2$ anatase surfaces. From the surface energies calculated using density functional theory (DFT) we derive the shape of the nanoparticles starting from the Wulff construction. Transmission electron microscopy (TEM) images of TiO$_2$ nanoparticles synthesized in non-aqueous medium show good agreement with the calculated shapes.

Invited Talk O 65.3 Wed 15:30 MA 005

Bulk-terminated surfaces of KTaO$_3$ and SrTiO$_3$ studied by combined STM/AFM — •Martin Setvin — TU Wien

Recent development of the noncontact atomic force microscopy (nc-AFM) has opened new possibilities in different fields - imaging of organic molecules [1], controlling the charge state of adsorbed species [2], or measuring forces involved in a single chemical bond [3]. I will focus on the possibilities and opportunities emerging on oxide surfaces. The limits of atomic resolution will be illustrated on clean and water-exposed binary oxides like TiO$_2$ or In$_2$O$_3$. The technique opens new ways towards investigation of complex oxides; this will be illustrated on the (001) surfaces of cubic perovskites KTaO$_3$ and SrTiO$_3$. These materials, when prepared by cleaving, consist of a mixture of two terminations (KO/TaO$_2$, SrO/TiO$_2$). The layout of these terminations resembles the shape of ferroelectric domains, indicating that the incipient-ferroelectric character of these materials can be used for tuning the surface topography. Basic physical and chemical properties of these surfaces will be discussed, with a special focus on the polar KTaO$_3$ (001) surface. This surface compensates its inherent instability by various mechanisms like formation of 2DEG-like states in the band gap, ferroelectricity, point defects, surface restructuring, or adsorbate-induced reconstruction. Tuning the environment allows choosing which mechanism will be in play and controlling the surface termination.

[1] L. Gross et al., Science 2009, 325, 1110 [2] L. Gross et al., Science 2009, 324, 1428 [3] Y. Sugimoto et al., Nature 2007, 446, 64

O 65.4 Wed 16:00 MA 005

On the role of strong metal-support interactions in the activity of Metal/CeO$_2$ catalysts — •M. Veronica Ganduglia-Pirovano[1] and Pablo G. Lustemberg[2] — [1]ICP-CSIC, Madrid, Spain — [2]IFIR-CONICET-UNR, Rosario, Argentina

Ceria (CeO$_2$) is the most significant of the oxides of rare-earth elements in catalysis. Specifically, the role of ceria in the catalytic activity of metal-ceria systems is still not fully understood. The non-innocent role of ceria as catalyst support will be analyzed using ceria-supported metal nanoparticles as experimental and theoretical model catalysts [1-4]. Co-, Ni- and Cu-ceria systems will be used for methane dry reforming ($CH_4+CO_2 \rightarrow 2H_2+2CO$), a relevant process from the environmental standpoint [1-3]. Ni-ceria will also be considered for hydrogen production [4]. The ability of ceria to stabilize oxidized species (Co^{2+} and Ni^{2+}) on the stoichiometric CeO$_2$ surfaces, by relocalizing electrons on localized f-states, and metallic ones (Co^0, Ni^0) on the reduced CeO_{2-x} support, is essential for catalytic activity.

[1] Z. Liu *et al.*, Angew. Chem. Int. Ed. 55, 7455 (2016).
[2] P. G. Lustemberg *et al.*, ACS Catal. 6, 8184 (2016).
[3] Z. Liu *et al.*, Angew. Chem. Int. Ed. 56, 13041 (2017).
[4] J. Carrasco *et al.*, Angew. Chem. Int. Ed. 54, 3917 (2015).

O 65.5 Wed 16:15 MA 005

Structural and electronic differences between tetragonal and monoclinic ZrO$_2$ films on Rh(111) — •Peter Lackner, Zhiyu Zou, Sabrina Mayr, Ulrike Diebold, and Michael Schmid — Institute of Applied Physics, TU Wien, Vienna, Austria

The applications of zirconia (ZrO$_2$) are manifold, e.g. as catalyst support or solid electrolyte in fuel cells. Despite the importance of the material, its surface has not yet been studied thoroughly on an atomic level. This has a simple reason: ZrO$_2$ has a band gap of more than 5 eV and is therefore non-conductive, which makes the study of bulk zirconia with methods like x-ray photoelectron spectroscopy (XPS) impracticable, and scanning tunneling microscopy (STM) close to impossible.

To circumvent this issue, we prepared five-monolayer-thick layers of ZrO$_2$(111) [1] on Rh(111) using a home-build UHV-compatible sputter source [2]. By annealing in $p_{O_2} = 10^{-6}$ mbar at $T < 700\,^\circ C$, we prepared tetragonal ZrO$_2$, while above 700 °C a phase transformation to monoclinic ZrO$_2$ – the stable bulk structure – was observed. Tetragonal ZrO$_2$ was atomically resolved, showing the expected (2×1) structure (w.r.t. cubic ZrO$_2$). The domain size grows with annealing temperature; at 650 °C, domains of $40 \times 40\,\mathrm{nm}^2$ are common. For monoclinic ZrO$_2$, a (2×2) structure was resolved. The two phases have distinct binding energies in the Zr3d region, with an unexpectedly high ΔE_B of 1.4 eV, pointing towards an unusual structure in one of the two.

[1] Meinel *et al.*, Phys. Rev. B 74, 235444 (2006).
[2] Lackner *et al.*, Rev. Sci. Instrum. 88, 103904 (2017).

O 65.6 Wed 16:30 MA 005

Structure and stability of the vicinal ZnO(10-14) surface — •Elin Grånäs[1], Björn Arndt[1,2], Marcus Creutzburg[1,2], Guilherme D.L. Semione[1,2], Heshmat Noei[1], Andreas Schaefer[3], Johan Gustafson[3], Vedran Vonk[1], and Andreas Stierle[1,2] — [1]Deutsches-Elektron Synchrotron (DESY), Germany — [2]University of Hamburg, Germany — [3]Lund University, Sweden

Zinc oxide (ZnO) based catalysts are commonly used, often together with Cu nanoparticles, in important chemical reactions such as methanol synthesis low temperature water-gas shift, and methanol steam reforming. ZnO plays not only the role as nanoparticle support; instead it is much more actively involved in many reactions, with detailed reaction mechanisms under discussion.

The commonly studied low index surfaces of ZnO are polar, resulting in surface instability, while the most stable surface has been suggested to be the vicinal ZnO(10-14) surface. However very little is still known about the equilibrium structure of the vicinal surface and its stability upon gas exposures. Here first studies performed on vicinal ZnO(10-14) single crystals will be presented. Using techniques such as scanning probe microscopy (STM), surface x-ray diffraction (SXRD), and x-ray photoelectron spectroscopy (XPS) we have characterized the bare and water exposed ZnO(10-14) surface. We have confirmed that the bare vicinal surface is stable in UHV and will discuss the atomic structure based on SXRD measurements. We will also discuss chemical and structural changes upon water exposure.

O 66: Plasmonics and nanooptics: Applications and other aspects II

Time: Wednesday 15:00–17:45 Location: MA 041

O 66.1 Wed 15:00 MA 041

Compact, Cheap, and Fully Optical Nanoplasmonic Gas Detection Scheme Demonstrated by Means of Hydrogen and CO_2 — •Tobias Pohl, Ediz Herkert, Florian Sterl, Nikolai Strohfeldt, and Harald Giessen — 4th Physics Institute and Research Center SCOPE, University of Stuttgart, D-70569 Stuttgart, Germany

Current gas detection systems are often bulky, expensive, and complex. Furthermore, many of these systems use electrical readout that poses a danger as possible ignition source. We introduce a novel general nanooptical gas detection scheme based on a plasmonic perfect absorber. The absorber, consisting of a mirror, a spacer layer and plasmonic disks, absorbs almost all light at a designed wavelength and can incorporate gas-sensitive materials to form a highly efficient detector. The fabrication method of colloidal etching lithography allows for cheap, large area, and mass production. We demonstrate the device capability through detection of hydrogen using palladium nanodisks and carbon dioxide by employing titanium dioxide as gas sensitive spacer layer. Incorporated into a custom-made compact sensing device with a simple combination of LED and photodiode, we studied the time-, concentration-, and temperature-dependent behavior of the fabricated sensor chips. In the future the generality of our platform will also enable us to expand its use to many different other gases by simply exchanging one material.

O 66.2 Wed 15:15 MA 041

Numerical modeling of second harmonic generation in metal nanoantennas — •Josselin Defrance and Thomas Weiss — 4th Physics Institute and Research Centers SCoPE, University of Stuttgart, Germany

Metallic nanoantennas can concentrate light into sub-wavelength volumes resulting in strong nonlinear responses. In order to understand and enhance this nonlinear optical phenomena, numerical methods play a crucial role. Different approaches have been developed to model the nonlinear interaction between the electromagnetic field and matter. The so-called Fourier modal method offers a fast and accurate calculation of far-field responses. It has been shown that the Fourier modal method can be extended in order to calculate the generation of higher harmonics [1,2]. However, convergence problems arise for complex geometries and at metal-dielectric interfaces. Therefore, we have combined this method with adaptive spatial resolution and matched coordinates [3] for calculating the nonlinear optical response of nanostructures with complex geometries. Furthermore, we will present our implementation of the hydrodynamic model in order to account for nonlocal contributions to the second-harmonic generation in metallic nanoantennas [4].

[1] T. Paul et al., J. Opt. Soc. B, Vol. 27, Issue. 5, pp. 1118 (2010).
[2] B. Bai et al., J. Opt. Soc. Am. B 24, pp. 1105-1112 (2007).
[3] T. Weiss et al., Opt. Express 17, pp. 8051 (2009).
[4] T. Paul et al., J. Mod. Opt. 58, 5-6, pp. 438-448 (2011).

O 66.3 Wed 15:30 MA 041

Large-area, disordered perfect absorber with multiple resonances in the visible and near infrared — •Ramon Walter and Harald Giessen — 4th Physics Institute, University of Stuttgart

Plasmonic devices with a very high absorption over a wide wavelength range, so-called perfect absorbers, have the potential for many applications as light trapping, photo catalysis and as black background for novel displays. Such systems show a very high absorption at their resonance, just by optimizing their impedance to vacuum values.

Such perfect absorbers can be fabricated on large-area scale, with low-cost, and a high throughput by using colloidal lithography, where nanospheres acting a mask for a dry-etching process. Due of the randomize dispersion of our nanostructures the absorption of the system remains very high over a wide range of incident angles, nearly independently of the polarization.

In this work, we investigate the potential of such devices for multiple resonances. Using nanospheres of different sizes should lead to various sizes of nanostructures and consequently to multiple resonances independently of the polarization. We investigate the interaction between two neighboring resonances in materials with different plasmonic characteristics, like e.g. gold or copper as typical plasmonic materials and nickel or palladium as representative *bad* plasmonic materials.

We believe that our investigations can lead to several designs with the potential for many applications. Systems with a high absorption over a width wavelength regime are also possible as reflectors for a narrow spectral area.

O 66.4 Wed 15:45 MA 041

Niobium as Alternative Material for Refractory Plasmonics and Hydrogen Sensing — •Shahin Bagheri[1], Nikolai Strohfeldt[1], Audrey Berrier[2], Michael Merker[3], Gunter Richter[4], Michael Siegel[3], and Harald Giessen[1] — [1]4 Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]1 Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany. — [3]Institute of Micro- and Nanoelectronic Systems, Karlsruhe Institute of Technology (KIT), Hertzstraße 16, 76187 Karlsruhe, Germany — [4]Max-Planck-Institut für Intelligente Systeme, D-70589 Stuttgart, Germany

Niobium is mainly known as a superconductive material, however, it exhibits similar plasmonic properties of noble metals such as gold. We utilize electron beam lithography combined with a plasma etching technique to fabricate nanoantenna arrays of Niobium. Tailoring of the Niobium antenna geometry enables precise tuning of the plasmon resonances from the near to the mid-infrared spectral range. The hydrogen absorptivity as well as high-temperature stability of the antennas has additionally been investigated. Great advantages of Niobium such as superconductivity, high-temperature stability, and hydrogen absorptivity, make Niobium highly attractive for plasmonic devices in the near future.

O 66.5 Wed 16:00 MA 041

Principal component analysis for SEIRA-based monitoring of structural changes in polypeptides — •Rostyslav Semenyshyn[1], Mario Hentschel[1], Jochen Vogt[2], Christian Huck[2], Christoph Stanglmair[3], Tanja Teutsch[4], Cristina Tarin[4], Claudia Pacholski[5], Harald Giessen[1], and Frank Neubrech[1,2] — [1]4th Physics Institute, University of Stuttgart, Germany — [2]Kirchhoff Institute for Physics, University of Heidelberg, Germany — [3]Max Planck Institute for Intelligent Systems, Stuttgart, Germany — [4]Institute for System Dynamics, University of Stuttgart, Germany — [5]Institute of Chemistry, University of Potsdam, Germany

Metal nanoantennas with plasmon resonances tuned to the infrared spectral region are perfectly suited for surface enhanced infrared absorption (SEIRA), which has already been applied to chemical analysis and biochemical sensing. Here, we demonstrate the capability of SEIRA for in-vitro observation of folding and unfolding processes of polypeptides monolayers by monitoring the enhanced amid vibrations of the molecules. As a model system, poly-L-lysine (PLL) was bond to the surface of gold nanoantennas utilizing a mixed monolayer of different thiols. We tuned the length of nanoantennas to be resonant at frequency of the amide-I band of PLL and performed SEIRA measurements in D_2O based solutions. To analyse the folding process, a principle component analysis (PCA) was applied. PCA is a powerful tool for tracking time evolutions in dynamic systems and is sensitive to slight changes. Applying this approach, we monitored the reversible folding and unfolding of PLL in ultra-low concentrations.

O 66.6 Wed 16:15 MA 041

Band structure engineered layered metals for low-loss plasmonics — •Morten Gjerding — DTU Physics, Fysikvej building 311, 2800 Kgs. Lyngby

Plasmonics currently faces the problem of seemingly inevitable optical losses occurring in the metallic components that challenges the implementation of essentially any application. In this work, we show that Ohmic losses are reduced in certain layered metals, such as the transition metal dichalcogenide TaS_2, due to an extraordinarily small density of states for scattering in the near-IR originating from their special electronic band structure. On the basis of this observation, we propose a new class of band structure engineered van der Waals layered metals composed of hexagonal transition metal chalcogenide-halide layers with greatly suppressed intrinsic losses. Using first-principles calculations, we show that the suppression of optical losses lead to improved performance for thin-film waveguiding and transformation optics.

15 min. break

O 66.7 Wed 16:45 MA 041

Geometry optimizaton of optical cavities and plasmonic resonators using quasinormal modes — •Philip Kristensen[1] and Kurt Busch[1,2] — [1]Institut für Physik - Humboldt-Universität zu Berlin, 12489 Berlin. — [2]Max-Born-Institut, 12489 Berlin.

Optical cavity modes and localized surface plasmon polaritons can be conveniently modeled by so-called quasinormal modes (QNMs), defined as the source free solutions to Maxwell's equations with the additional requirement of a radiation condition. The QNMs capture most - if not all - the properties typically expected from open electromagnetic resonators. In particular, the radiative loss and material absorption result in complex resonance frequencies, from which the quality factors Q can be calculated directly. From a modeling perspective, one can use perturbation theory with QNMs to estimate the change in resonance frequency due to small changes in the material making up the resonator. In this work, we present a geometry optimization algorithm for controlled tuning of electromagnetic resonators. At each step of the algorithm, we use QNM perturbation theory to calculate the optimum variational change in the resonator boundary required to iteratively shift the complex resonance frequency towards a desired value. This approach alleviates the need for extensive variational testing at each iteration step and provides a stable and efficient overall improvement of the optimization metric. The resulting resonators show interesting and non-trivial organic shapes and support QNMs with optimized parameters, such as increased Q factors.

O 66.8 Wed 17:00 MA 041

Applications of plasmonic standing waves — Petr Dvořák, Michal Kvapil, Zoltán Édes, Petr Bouchal, Tomáš Šamořil, •Vlastimil Křápek, and Tomáš Šikola — CEITEC, Brno University of Technology, Purkyňova 123, CZ 61200 Brno, Czech Republic

We demonstrate formation of plasmonic standing waves on top of a gold layer. Subwavelength slits fabricated in the gold layer by focused ion beam milling serve as sources of propagating surface-plasmon-polariton waves when illuminated from bottom. By proper arrangement of the slits it is possible to form a desired interference pattern, which is then imaged using scanning near-field optical microscopy (SNOM).

We demonstrate several applications of the plasmonic standing waves. (1) We performed spectroscopic measurements of plasmon interference patterns by an aperture-type SNOM setup equipped with a supercontinuum laser and a polarizer. The series of wavelength- and polarization-resolved measurements, together with results of numerical simulations, then allowed us to identify the role of individual near-field components (in-plane, out-of-plane) in formation of SNOM images [1,2]. (2) We demonstrate (plasmo)luminescence of optical emitters located near the interference maxima. (3) Using spatial light modulator to modify the phase of the wave illuminating the slits we are able to reconstruct the phase of the plasmonic standing wave.

[1] P. Dvořák *et al.*, Nano Lett **13**, 2558 (2013).
[2] P. Dvořák *et al.*, Opt. Express **25**, 16560 (2017).

O 66.9 Wed 17:15 MA 041

Electroluminescence from optical Yagi-Uda antennas — •Maximilian Ochs, René Kullock, Philipp Grimm, Monika Emmerling, and Bert Hecht — NanoOptics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

Light-based on-chip communication promises much higher data transfer rates than conventional electrical circuitry. One promising approach is the use of directional antennas, e.g. Yagi-Uda antennas which are very common in the radio frequency regime. Downscaling these systems to nanometer size would enable directional radiation of light, however, since for these frequencies no conventional electrical generators exist, so far they have only been driven optically [1].

Here, we demonstrate electrically-driven optical Yagi-Uda antennas based on dipole antennas [2], radiating directional with FB-ratios of around 5 dB. Light emission is facilitated by the quantum shot noise of electrons tunneling across the antenna gap upon applying a voltage. The presented fabrication yields a high reproducibility and we show that the directivity as well as the properties of the electroluminescence can be controlled by the antenna geometry. Our work paves the road for wireless communication on the nanometer scale between a set of individual antennas.

[1] A. Curto et al.,*Science 329, 5994 (2010)*
[2] J. Kern et al.,*Nat. Photonics 9, 9 (2015)*

O 66.10 Wed 17:30 MA 041

Influence of surface plasmons on energy dissipation in laser-excited materials — •Pavel N. Terekhin[1,2], Sebastian T. Weber[1], and Baerbel Rethfeld[1] — [1]Department of Physics and Research Center Optimas, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany — [2]National Research Centre "Kurchatov Institute", Kurchatov Sq. 1, 123182 Moscow, Russia

In our work we simulate the excitation and decay of surface plasmons during and after ultra-short laser irradiation. In our sample system, surface plasmons can be created in two different ways: at an interface between an absorbing metal and a dielectric coating as well as at edges and defects of a metal surface.

We want to take into account the field enhancement of the electrical field resulting from the surface plasmons. Then, we extend the two-temperature model (TTM) to describe the interaction of hot electrons with an additional plasmon subsystem. The aim is to obtain the time evolution of the energy transfer between plasmons, electrons and the crystal lattice. Our approach will shed light on the fundamental mechanisms of the materials' excitation, and, additionally, it will give promising perspectives for the technological controlling of the nanostructuring of material surfaces.

O 67: Electronic structure of surfaces: Spectroscopy, surface states III

Time: Wednesday 15:00–18:00 Location: MA 042

Invited Talk O 67.1 Wed 15:00 MA 042

Ultrafast dynamics of two-dimensional electron systems probed by time- and angle-resolved two-photon photoemission — •Jens Güdde — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, 35032 Marburg

Two-dimensional (2D) electron systems have attracted interest for more than 40 years due to unique properties that have no counterpart in 3D. In this talk I will first report on a 2D electron gas with close to ideal properties for fundamental studies. Ultrathin He films on single-crystal metal surfaces allow for an isolation of the electron system from the bulk and at the same time achieve a relatively large binding energy due to a strong image-force interaction with the metal. Our results for a monolayer (ML) of He/Cu(111) let us extrapolate lifetimes of nanoseconds for only a few ML of He on substrates such as Cu(100) with binding energies that are still large enough to support electron densities up to the quantum regime without instabilities [1].

Topologically protected states at the surfaces of 3D topological insulators represent a model for relativistic 2D electron systems with a characteristic Dirac-like energy dispersion. Optical excitation with near-infrared light pulses offers the possibility to induce and control spin-polarized electrical surface currents without exciting the bulk electron system [2]. Our experiments reveal unusually long elastic decay times of these currents due to spin-momentum locking of the Dirac electrons.

[1] N. Armbrust *et al.* Phys. Rev. Lett. **116**, 256801 (2016).

[2] K. Kuroda *et al.*, Phys. Rev. Lett. **116**, 076801 (2016).

O 67.2 Wed 15:30 MA 042

Light-molecule interactions in plasmonic environments — •Emiliano Cortes — Physics Department, Imperial College London, UK

Unravelling the interaction of single molecules with plasmonic interfaces sets the basis for plasmonic chemistry. Enhanced electric fields, energetic (hot) electron-hole pairs and abrupt thermal gradients, build up a complex scenario for molecules sitting next to a metal nanoparticle illuminated at visible wavelengths. However, at the same time, this combination offers all the necessary ingredients to manipulate photochemical reactions and ultimately revolutionize the electromagnetic-into-chemical energy conversion processes. In this context, single molecule and/or single nanoparticle approaches, even being methodologically challenging, should reduce the complexity of the problem allowing to explore, rationalize and optimize energy transfer pathways in these systems. Here, I will show a range of examples where the energy confinement achieved by plasmonic nanoparticles has been further employed to in-situ monitor, guide or induce charge-transfer processes at the single molecule and/or the single nanoparticle level. Using light to study, enhance and drive chemical reactions, beyond the traditional photochemistry or photocatalysis fields, is now possible thanks to plasmonic chemistry.

O 67.3 Wed 15:45 MA 042

Electronic structure of LAO/STO thin films: artificial control of the quantum well states or enhanced polaronic tail? — •Marco Caputo[1], Alessio Filippetti[2], Margherita Boselli[3], Alla Chikina[1], Hugo Dil[4], Claudia Cancellieri[5], Stefano Gariglio[3], Jean-Marc Triscone[3], and Vladimir N. Strocov[1] — [1]Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen-PSI, Switzerland — [2]CNR-IOM, Istituto Officina dei Materiali, Cittadella Universitaria, Cagliari, Monserrato 09042-I, Italy. 7 — [3]DPMC, University of Geneva, 24 Quai Ernest Ansermet, 1211 Geneva, Switzerland — [4]Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — [5]EMPA, Swiss Federal Laboratories for Materials Science & Technology, Ueberlandstrasse 129, CH-8600 Duebendorf, Switzerland

Transition Metal Oxides (TMO) represent an ideal platform to exploit exotic phenomena in solid state physics. Conductivity and superconductivity in the 2D Electron System (2DES) at the LAO3/STO3 (LAO/STO) interface is one of them.

The 2DES sits on the STO part of the interface, in a potential well created by band bending. Reducing the thickness of the hosting STO material can provide a platform for new exotic phenomena, like quantum well states.

In this work we analyze the electronic structure of a LAO/STO interface, where the STO side was a thin layer of few unit cells grown on a LAO layer deposited on a STO substrate.

O 67.4 Wed 16:00 MA 042

Optical anisotropy of SrTiO$_3$(110) for different surface terminations — •Karsten Fleischer, Brian Walls, Kuanysh Zhussupbekov, and Igor V. Shvets — School of Physics, Trinity College Dublin, The University of Dublin, Dublin 2, Ireland

In this work we investigate the SrTiO$_3$(110) surface by reflectance anisotropy spectroscopy (RAS) at varying preparation steps including ex-situ wet etching, high temperature oxygen annealing, as well as in-situ vacuum annealing. Different surface terminations show distinctly different RAS spectra which are correlated to an altered surface stoichiometry measured by X-ray photoelectron spectroscopy (XPS) and an altered valence band structure measured by UV-photoelectron spectroscopy (UPS) in cases of conductive samples. We link the changes in the observed RAS spectra to various surface reconstructions, with particular focus of the signature of (3×1) and (1×4) reconstructed surfaces, and a metallic surface state observed in vacuum annealed SrTiO$_3$.

O 67.5 Wed 16:15 MA 042

Revealing the Wave Nature of Hot Electrons with a Molecular Nanoprobe — •Markus Leisegang[1], Jens Kügel[1], Lucas Klein[1], and Matthias Bode[1,2] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Wilhelm Conrad Röntgen Center of Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg

Electron transport in materials is usually determined by conductance measurements performed in between two contacts which are typically separated by a minimal distance of hundreds of nanometers. Future nanoscale applications like single-molecule logic gate structures [1], however, will require characterization of transport properties on much shorter length scales. Here we show how STM-induced molecular nanoprobing (MONA) can be used for the characterization of quasiparticle transport on a length scale well below 10 nanometer [2]. We present results obtained on dehydrogenated H$_2$Pc molecules. Isomerization was triggered by hot electrons injected from a STM tip into the Ag(111) substrate close to the molecule. By utilizing various atom-by-atom–engineered Ag nano structures we are able to determine how quasiparticles propagate and under which conditions interference of coherent quantum-mechanical wave functions are observed. We will show how these findings can be utilized to create an energy-selective filter for single-molecule switches.

[1] C. Li *et. al.*, Nature Nano. **12**, 1071-1076 (2017)

[2] J. Kügel *et. al.*, Nano Lett. **17**, 5106-5112 (2017)

15 min. break

O 67.6 Wed 16:45 MA 042

First-principles modeling of secondary electron emission from slow ion bombardment — •Marnik Bercx, Bart Partoens, and Dirk Lamoen — EMAT & CMT groups, Department of Physics, University of Antwerp

Secondary electron emission (SEE) is an important phenomenon where electrons of a target material are emitted through the impact of energetic (primary) particles. Such processes lie at the foundation of several techniques for characterizing materials and play an important role in applications such as plasma sputtering deposition or plasma display panels. In our work, we start from the pioneering work of Hagstrum [1] to construct a quantitative model that allows for the determination of the SEE yield from slow ions incident on a surface. We provide a fully ab initio approach by calculating the required input from first-principles Density Functional Theory calculations, as well as making some major conceptual improvements to the model. We further expand the model to include plasmon excitations, which are believed to have a significant effect on the yield spectrum for materials with low plasmon frequencies [2]. The calculated yield spectra, i.e. the kinetic energy distribution of the emitted electrons, are in excellent agreement with experimental results for several semiconductors (Ge, Si) and metals (Al, Mg, Be).

O 67.7 Wed 17:00 MA 042

First-principles study on the bulk and surface Rashba states of GeTe — •Jaemo Lihm and Cheol-Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea

GeTe displays giant bulk and surface Rashba-type spin splitting as a result of its ferroelectric polarization and strong spin-orbit coupling [1,2]. The energy and spin polarization of the bulk and surface Rashba states of GeTe has been closely studied both theoretically and experimentally, due to its potential in the external control of electron spin [3]. In this presentation, we report the results of our first-principles study on the electronic structure of bulk and surface Rashba split bands using density-functional-theory calculations. We find the different roles of broken inversion symmetry and the spin-orbit coupling in the Rashba effect of GeTe. The bulk-surface resonance effect brings about complexity in the electronic structure of the surface Rashba states. The effects of potassium adsorption on the surface Rashba states are also investigated.

[1] D. Di Sante et al., Adv. Mater. 25, 509-513 (2013)
[2] M. Liebmann et al., Adv. Mater. 28, 560-565 (2016)
[3] J. Krempaský et al., arXiv:1707.08431 (2017)

O 67.8 Wed 17:15 MA 042

Giant Rashba Splitting in Cu_2Te and Ag_2Te Surface Alloys — •Maximilian Ünzelmann[1], Hendrik Bentmann[1], Dean Nestorov[1], Philipp Eck[2], Domenico Di Sante[2], Giorgio Sangiovanni[2], Philipp Rosenzweig[3], Sebastian Otto[3], Thomas Fauster[3], and Friedrich Reinert[1] — [1]Experimentelle Physik 7, Universität Würzburg — [2]Theoretische Physik 1, Universität Würzburg — [3]Lst. f. Festkörperphysik, Universität Erlangen-Nürnberg

By deposition of a 1/3 ML of Tellurium on M(111) surfaces (M=Cu,Ag) a $(\sqrt{3}\times\sqrt{3})$-R30° superstructure in M_2Te stoichiometry is formed whereby every third M-atom is replaced by a Te-atom. This type of substitutional surface alloys is very well known as a model system for large Rashba-type spin-orbit splittings.
We investigated the surface band structure of $M_2Te/M(111)$ by means of one- and two-photon photoelectron spectroscopy and compare our photoemission data to density functional theory (DFT) band structure calculations. For both substrates two fully occupied hole-like bands are found. We assign these to Te induced sp_z- and p_xp_y-states. Our ARPES data shows strong indications for a Rashba-type spin splitting with a Rashba parameter of about 2 eVÅ for the Ag_2Te sp_z-state. Interestingly this value is much larger than that for Sb which has a similar atomic SOC. This manifests the influence of the atomic structure on the Rashba spin splitting. Besides a series of image-potential-resonances 2PPE shows Te-induced unoccupied states in good agreement with DFT calculations.

O 67.9 Wed 17:30 MA 042

First-principles calculations on the surface states of KHgSb: hourglass fermions — •Ji Hoon Ryoo and Cheol-Hwan Park — Department of Physics & Astronomy, Seoul National University 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea

It has been recently proposed [1] and experimentally confirmed [2] that exotic surface states reside in the surface of KHgSb, so-called hourglass fermions named after their peculiar energy band structure. In this contribution, we present the results of our comprehensive first-principles study on the electronic structure of KHgSb surface and bulk. Especially, we highlight the role of spin-orbit coupling and symmetry on the spin texture of these hourglass fermions.

[1] Z. Wang, A. Alexandradinata, R. J. Cava, B. A. Bernevig, Nature 532, 189 (2016).
[2] J. Ma et al., Science Advances 3, e1602415 (2017).

O 67.10 Wed 17:45 MA 042

Density-Functional Theory based calculation of core-level spectroscopies: Transition and Rare Earth Metals — •Georg S. Michelitsch and Karsten Reuter — Technische Universität München

Core-level spectroscopies are among the most established methods of characterization in modern material science, providing information about chemical interactions and the environment of an atomic species in a composite material matrix. A reliable interpretation of experimental signatures often requires support by computational spectroscopy. Parametrized, effective models are in most cases sufficient to explain main features or isolated resonances based on general assumptions of ligand field theory. Overlapping resonances and strong chemical shifts due to interatomic bonding instead demand an explicit calculation of the intricate electronic structure from first principles. For extended systems, the latter generally translates to density-functional theory (DFT), relying on an approximate treatment of core-hole screening via occupational constraints. While established and highly successful for light elements, this approach is challenged by transition and rare earth metals with their partially filled *d*- and *f*- states, where relativistic effects and strong local Coulomb repulsion need to be appropriately described. We assess this situation through DFT calculations for hybrid organometallic materials incorporating transition and rare earth metals with an emphasis on the impact of the chemical environment on the X-ray signatures. We find good agreement with experiment already at the level of perturbative spin-orbit coupling.

O 68: Surface dynamics: Reactions, elementary processes and phase transitions I

Time: Wednesday 15:00–16:30 Location: MA 043

O 68.1 Wed 15:00 MA 043

2-Dimensional Vibrational Sum Frequency Generation Spectroscopy of Organic Monolayers — •Anna K Schiffer, Mike Hemsworth, and Gary W Leach — Simon Fraser University, Chemistry Department, Laboratory for Advanced Spectroscopy and Imaging at 4D Labs, Burnaby, BC, Canada

Vibrational sum frequency generation (SFG) spectroscopy is a non destructive interface-specific non linear optical spectroscopy that delivers information about the structure and composition of interface environments. SFG spectroscopy leverages the non centrosymmetric environment of the interface to mix two incident electric fields and provide a coherent scattered field at the sum of incident frequencies. If one of the fields is resonant with the vibrational modes of interface molecules, the sum frequency signal will provide information about the local interface structure. The extension to a 2-dimensional (2D-SFG) spectroscopy provides direct information about the interactions between molecules and their dynamics at the interface by employing pulse sequences. Here, we describe the construction of a collinear 2D-SFG spectrometer and its application to the vibrational spectroscopy of highly ordered organic monolayers at the CaF2/Air interface. A three pulse IR sequence is generated by using a dual output optical parametric amplifier (OPA) pumped by an amplified Ti:sapphire laser system and a pair of birefringent wedges. The wedges create a highly phase stable pair of IR pulses with controllable time delays. The signals are subsequently processed to provide 2D-SFG spectra and provide information about the dynamics of the sample in the CH spectral region.

O 68.2 Wed 15:15 MA 043

Analyzing and Tuning the Energetic Landscape of H_2Pc Tautomerization — •Lucas Klein[1], Jens Kügel[1], Markus Leisegang[1], and Matthias Bode[1,2] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Wilhelm Conrad Röntgen Center of Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg

Many chemical and biological reactions are associated with the quantum tunneling of hydrogen atoms through a potential barrier in the reaction path [1]. Whereas quantum tunneling is often identified by temperature-dependent measurements or a large kinetic isotope effect, we demonstrate a new method working at a fixed temperature. As a model system we used the tautomerization—the switching of hydrogen protons between different adsorption sites—of phthalocyanine (H_2Pc) molecules adsorbed on a Ag(111) surface which are probed by scanning tunneling microscopy. We will show, that the tautomerization of this molecule is exclusively triggered by the excitation of the N–H stretching mode. Interestingly, a step-like increase of the tautomeriza-

tion rate is observed at a bias voltage that corresponds to the second harmonic of this vibrational mode, which we attribute to a crossover from quantum tunneling through the tautomerization barrier to an excitation over the barrier. This explanation is further supported by modifying the energetic landscape of the tautomerization of pristine H_2Pc by single silver atom manipulation and/or deprotonation.
[1] M. Koch *et. al.*, J. Am. Chem. Soc. **139**, 12681-12687 (2017)

O 68.3 Wed 15:30 MA 043

Free energy landscape of graphene surface reactions from ab initio simulations — •Mateusz Wlazlo and Jacek Majewski — Faculty of Physics, University of Warsaw, Poland

We study methane (CH_4) and carbon dioxide (CO_2) decomposition and adsorption processes on monolayer graphene. These classes of reactions are important in chemical vapor deposition (CVD) growth of graphene or in CH_4-CO_2 exchange reactions, for example. The occurrence of this exchange is advantageous in the removal and storage of atmospheric CO_2.

The studies are based on *ab initio* molecular dynamics methods implemented in the framework of planewave density functional theory. Free energy profiles featuring energy barriers for different steps of the reaction are computed using the so-called *Blue Moon ensemble* method. The barriers are much lower than experimental bond dissociation energies for gaseous species, strongly indicating that graphene surface acts as a catalyst of decomposition reactions. However, the barriers are still much higher than on nickel surface. This suggests that monolayer formation should be favored over multilayer graphene, which reinforces the position of nickel as a suitable substrate for large-scale, high-quality CVD graphene growth.

Calculations show different preferred mechanisms of CH_4 and CO_2 adsorption, depending on surface morphology. On ideal graphene, dissociative adsorption is preferred whereas on defect sites, such as the Stone-Wales defect, direct chemisorption of CO_2 occurs with higher likelihood.

O 68.4 Wed 15:45 MA 043

Femtosecond laser-induced associative desorption of molecular hydrogen from graphite — •Lorenzo Maddii Fabiani, Robert Frigge, John Thrower, and Helmut Zacharias — Physikalisches Institut, Westfälische-Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Deutschland

The formation of molecular hydrogen via radiation-induced associative desorption from dust particles may play an important role in photon dominated regions of the interstellar medium. In this study we investigate the desorption of molecular hydrogen and deuterium from HOPG following surface excitation with fs-laser pulses at $\lambda = 400$ nm. Desorbed neutral species are analyzed by internal state selective two-photon ionization (1+1) REMPI in the XUV region.

The desorbing hydrogen molecules show strongly non-equilibrium state populations. The vibrational ground state is less populated than the first excited one, while measurements for higher vibrational states are on-going. State specific kinetic energy measurements result in a value for $v'' = 1$, $E_{kin} = 100$ meV, significantly lower than for $v'' = 0$, $E_{kin} = 170$ meV. The rotational populations present a non-thermal distribution that can be fitted by two rotational temperatures for low and high J''. The average rotational energy is determined to $E_{rot} = 390$ cm^{-1} for $v'' = 0$ and 480 cm^{-1} for $v'' = 1$. A nonlinear fluence dependence of the desorption yield allows two-pulse correlation measurements, which give an insight into the relevant desorption mechanisms. The FWHM of ca. 450 fs suggests an electron induced desorption mechanism.

O 68.5 Wed 16:00 MA 043

Water formation reaction physically confined below silica thin films: real time observation using LEEM and PEEM — •Mauricio Prieto[1], Hagen Klemm[1], Feng Xiong[2], Daniel Gottlob[1], Dietrich Menzel[1], Thomas Schmidt[1], and Hans-Joachim Freund[1] — [1]Department of Chemical Physics, Fritz Haber Institute of the Max Planck Society. Berlin - Germany — [2]Department of Chemical Physics, University of Science and Technology of China, Hefei - P. R. China.

Thin oxide films are interesting models for the studying fundamental properties of real catalysts [1]. Among the more studied oxides, silica has caught the attention due to its relevance in the field of heterogeneous catalysis as a support or active component [2]. In addition, silica thin films supported on Ru(0001) have shown the ability of intercalating molecules into the confined space existing between the crystal surface and the oxide film [3]. We will show results regarding the study of the hydrogen oxidation with the aberration corrected spectromicroscope SMART [4] at the synchrotron light source BESSY-II in Berlin, by means of local XPS, LEED and LEEM. For instance, the reaction occurs as a front characterized by a sudden change in intensity in LEEM. The apparent activation energy of the process could be evaluated and compared with data obtained for bare Ru(0001), thus addressing the effect of confinement on the chemical reaction.

[1] Libuda, et al., Microchim. Acta 156, 9 (2006) [2] Ulrich, et al., Phys. Rev. Lett. 102, 016102 (2009) [3] Emmez, et al.; J. Phys. Chem. C 118, 29034 (2014) [4] Schmidt, et al., Ultram. 110 1358 (2010)

O 68.6 Wed 16:15 MA 043

Electron-mediated phonon-phonon coupling drives the vibrational relaxation of molecules at metal surfaces — •Dino Novko[1], Maite Alducin[2,4], and Joseba Iñaki Juaristi[2,3,4] — [1]Freie Universität, Institut für Chemie und Biochemie, Berlin — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), San Sebastián, Spain — [3]Departamento de Física de Materiales, Facultad de Químicas UPV/EHU, San Sebastián, Spain — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain

Growing experimental evidences highlight a key role of nonadiabatic coupling in adsorbate relaxation at metal surfaces. Even though many nonadiabatic theories have emerged to comprehend these experimental endeavours, our understanding of the microscopic mechanisms that underlie the dynamical processes at metal surfaces is still incomplete. For instance, the state-of-the-art theories are still unable to give precise quantitative estimations of the experimental vibrational relaxation rates. In this contribution we propose a new relaxation process, i.e., the so-called electron-mediated phonon-phonon coupling (EMPP), that is able to elucidate the vibrational relaxation mechanism of the internal stretch mode of CO on Cu(100). In fact, we show that the EMPP process dominates over the commonly-used first-order nonadiabatic contribution. The results demonstrate a strong electron-mediated coupling between the internal stretch and low-energy CO modes, but also a significant role of the surface motion. Our nonadiabatic theory is also able to explain the temperature dependence of the internal stretch phonon linewidth, thus far considered a sign of the direct anharmonic coupling.

O 69: Nanostructures at surfaces: 1D and 2D structures and networks II

Time: Wednesday 15:00–16:30 Location: MA 141

O 69.1 Wed 15:00 MA 141

Graphene nanoribbons on gold: superlubricity and edge effects — •Lorenzo Gigli — SISSA (International School of Advanced Studies), Via Bonomea 265, Trieste (TS), Italy

Via numerical simulations, we investigate the static structural features and the frictional response of n = 7 armchair graphene nanoribbons (GNRs) of different lengths deposited on a gold Au(111) substrate, a tribological interface subject of recent, intense experimental studies. The C-Au lattice mismatch and the GNR-substrate relative orientation dictate the periodicity of the interface Moire' pattern for the relaxed GNR configurations. By adiabatically increasing an uniform external force directed along the longitudinal GNR axis, the molecular-dynamics approach shows a static frictional response which does not grow with the GNR length, thus supporting the experimental data of a superlubric behavior with negligible frictional contribution of the internal bulk region of the ribbon. The peculiar oscillatory trend of the static friction versus length, around a fairly constant mean value (tens of pN), correlates with the characteristic modulation of the observed Moire' pattern (2D Materials 4, 045003, 2017).

Mimicking the experimental framework by Kawai et al. (Science 351, 957, 2016), we also present results of the dynamical response of deposited GNRs, lifted at one end and pulled laterally by a spring moving at constant velocity. Competition between peeling and sliding mechanisms, stick-slip and smooth dynamics are discussed in terms of the edge-lifting height and the effective GNR elasticity.

O 69.2 Wed 15:15 MA 141

Reaction pathway towards 7-armchair GNR formation and identification of intermediate species on Au(111) — Sebastian Thussing, •Sebastian Flade, and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

The reaction pathway of 10,10'-dibromo-9,9'-bianthryl (DBBA) deposited onto Au(111), eventually leading to the formation of 7-armchair graphene nanoribbons (7-AGNR) has been investigated. Individual reaction steps, along with the respective reaction intermediates were identified using IR-absorption and thermal desorption spectroscopy. They are characterized by distinct molecular species which have undergone (i) halogen abstraction, (ii) polymerization of the bianthryl units, (iii) H-abstraction and 5^+-AGNR formation, and (iv) further H-abstraction and 7-AGNR formation. Identification of surface species is aided by calculations of the vibrational properties of various model compounds. Comparison of TDS and IRAS data allows us to establish a correlation between individual surface reaction steps and processes leading to the desorption of molecular species, e.g. of intact DBBA, HBr, and H_2. Our refined model fully corroborates earlier observations of intermediate stages in the 7-AGNR formation using STM [1, 2].

[1] J. Cai et al., Nature 466 (2010) 470. [2] S. Blankenburg et al., ACS Nano 6 (2012) 2020.

O 69.3 Wed 15:30 MA 141

Magnetism in narrow graphene ribbons: open shells and quantum fluctuations — •Richard Korytár — Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Graphene-type carbon structures are very frequently discussed for spintronics applications. These structures can host intriguing physical phenomena, such as electronic zero modes and localized spin states, with high relevance for the transport of spin and charge. I address some of these features in a prototypical example, the linear oligoacenes, which are the narrowest zig-zag graphene flakes. The importance of electron-electron interactions can not be underestimated as it underlies the effects such as edge-states or poly-radicals. I will examine the role of interactions by constructing an acene-like Hubbard model. The physics of non-interacting electrons manifests by peculiar oscillations of the excitation gaps with molecular length. The role of electron-electron interactions will be explored by comparing two approaches: an unrestricted Hartree-Fock and a numerically exact DMRG solution. Quantum fluctuations wipe out spin-polarized states and restore the band-structure effects in a large portion of the parameter space.

Wang, S. and Talirz, L. and Pignedoli, C. A. and Feng, X. and Müllen, K. and Fasel, R. and Ruffieux, P. Nature Communications 7, 11507 (2016)

P. Schmitteckert, R. Thomale, R. Korytár and F. Evers, The Journal of Chemical Physics 146, 092320 (2017)

R. Korytár, D. Xenioti, P. Schmitteckert, M. Alouani, F. Evers, Nature Communications 5 5000 (2014)

O 69.4 Wed 15:45 MA 141

Polymer Adsorption on Individual Single-Wall Carbon Nanotubes — •Matthias Josef Kastner[1] and Tobias Hertel[1,2] — [1]Institut für Physikalische und Theoretische Chemie, Julius-Maximilians-Universität Würzburg, Germany — [2]Röntgen Center for Complex Material Systems, Julius-Maximilians-Universität Würzburg, Germany

Polyfluorene copolymers are frequently used for the chirality-specific isolation of individualized Single-Wall Carbon Nanotubes (SWNTs). The interaction of polymers such as PFO-BPy with the carbon nanotube surface thus plays a key role in providing the desired selectivity. The objective of this work is to better understand and study the adsorption of single polymer strands on the SWNT surface by fluorescence microscopy and spectroscopy.

In the approach presented here we are using individual SWNTs, freely suspended across micron-sized trenches of a patterned SiO2 substrate and immersed in organic solvent. The adsorption of PFO-BPy is here monitored using changes in the intensity and center wavelength of SWNT exciton photoluminescence from individual nanotubes as a very sensitive probe for changes at the SWNT-solvent interface. Understanding of such adsorption processes is expected to lead into new insights which can be used for the chemical design of new selective polymers.

O 69.5 Wed 16:00 MA 141

Dependence of the adsorption height of graphene-like adsorbates on their dimensionality — •Serguei Soubatch[1], Simon Weiss[1], Xiaosheng Yang[1], Arnulf Stein[2], David Gerbert[2], Christine Brülke[3], Roman Kremring[3], Sascha Feldmann[2], Alex Schenk[4], Marie Gille[5], Timo Heepenstrick[3], Ina Krieger[3], Francois Bocquet[1], Stefan Hecht[5], Moritz Sokolowski[3], Petra Tegeder[2], and Stefan Tautz[1] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany — [3]Universität Bonn, Bonn, Germany — [4]La Trobe University, La Trobe, Australia — [5]Humboldt-Universität zu Berlin, Berlin, Germany

We measured the adsorption height of various graphene nanoribbons on the Cu(111) and the Au(111) surfaces and hexagonal boron nitride (hBN) and graphene on the Cu(111) surface using the x-ray standing waves technique. On Au(111), the different types of nanoribbons studied in our work are found to be physisorbed, while on Cu(111) the adsorption height is noticeably reduced pointing at a significant contribution of chemical interactions. Comparing to π-conjugated molecules on the one hand and hBN and graphene on the other, we observe a strong dependence of the adsorption height on the dimensionality of the adsorbate. This shows that graphene-like carbon adsorbates interact with the metal substrate mainly via the electron density of the honeycomb lattice. Chemical interactions involving edge atoms play a minor role.

O 69.6 Wed 16:15 MA 141

Light assisted charge spreading and charge trapping in organic semiconductors needles supported by 2D materials — •Aleksandar Matković[1], Markus Kratzer[1], Jakob Genser[1], Daniel Lüftner[2], Peter Puschnig[2], Zhongrui Chen[3], Olivier Siri[3], Conrad Becker[3], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben, Franz Josef Strasse 18, 8700 Leoben Austria — [2]Institute of Physics, University of Graz, NAWI-Graz, Universitätsplatz 5. 8010 Graz, Austria — [3]Aix Marseille Université, CNRS, CINaM UMR 7325, 13288 Marseille, France

In this study we investigate the growth of an oligoacene derivate dihydrotetraazaheptacene (DHTA7), which - due to nitrogen containing groups - forms solids through H-bonding and dipolar interactions between neighboring molecules. As a result of H-bonding networks, the molecules form in-plane rows with subsequent layers exhibiting π-π stacking. Crystalline needles of DHTA7 were grown by hot wall epitaxy on the surfaces of graphene and hexagonal boron nitride, which act as van der Waals electrodes and gate dielectrics. Using photo-assisted electrostatic force microscopy we demonstrate charge trapping and light-assisted charge spreading within the networks of DHTA7 needles. We found that in the dark these needles are not conductive, while visible light linearly polarized parallel to the long axis of the needles allows spreading of the charges across the network for tens of micrometers. Results indicate that - due to the inverse population created by the laser - charges that were trapped in the localized defects can spread through the bands of the organic semiconductor.

O 70: Solid-liquid interfaces: Reactions and electrochemisty III (joint session O/CPP)

Time: Wednesday 15:00–16:15 Location: MA 144

O 70.1 Wed 15:00 MA 144

Atomically-Defined Pt/Co_3O_4(111) as Model Electrocatalyst — •Manon Bertram, Corinna Stumm, Firas Faisal, Yaroslava Lykhach, Olaf Brummel, and Jörg Libuda — Physikalische Chemie II, FAU Erlangen

The surface science approach, i.e. studying model catalysts in ultra-high vacuum (UHV), is well known in heterogeneous catalysis. We apply this approach to electrocatalysis and transfer complex, but well-defined catalysts from UHV to electrochemical (EC) conditions.

As a model system we prepared Pt nanoparticles (NPs) on ordered Co_3O_4(111) thin films on Ir(100). The oxide support and the complete catalyst were characterized by low-energy electron diffraction (LEED), x-ray photoelectron spectroscopy (XPS) and other methods. We transferred the systems to EC environments under ultra-clean conditions. With a scanning flow cell coupled to an inductively coupled plasma mass spectrometer and EC infrared reflection-absorption spectroscopy (EC-IRRAS), LEED, and XPS we determined the stability window for the oxide support under EC conditions.

Using Pt/Co_3O_4(111) with different Pt loadings, we followed the CO electro-oxidation by EC-IRRAS and cyclic voltammetry. As reference, we studied CO adsorption under UHV conditions with infrared reflection absorption spectroscopy. We identify different adsorption sites, a suppression of bridging CO on small NPs, and electronic metal support interactions (EMSI) leading to formation of partially oxidized Pt. The EMSI influences the CO adsorption and, thus, the electrocatalytic properties.

O 70.2 Wed 15:15 MA 144

Real-Time Measurement of Silica Dissolution at the interface with water — •Jan Schaefer, Ellen H.G. Backus, and Mischa Bonn — Max Planck Institute for Polymer Research, Mainz, Germany

Dissolution processes of minerals in water are often studied on macroscopic scales by detecting dissolution products in bulk solution and inferring microscopic reaction rates using models that require assumptions. Here, we present a direct way to measure the dissolution rate of silica, a mineral of geological significance, in contact with water. We find that on a surprisingly short timescale of tens of hours, the interfacial concentration of dissolution products saturates at a level close to the solubility of silica (~ millimolar). As the bulk solution is known to be equilibrated only after several weeks, our results reveal that the macroscopic dissolution process is limited by diffusion. A comparison with a simple 1D reaction/diffusion model indicates that the diffusion coefficient of dissolved silica decays with progressing dissolution which suggests that the small silicic acid species polymerize next to the silica surface.

O 70.3 Wed 15:30 MA 144

Charge transfer across the n-GaP(100) photoanode/electrolyte interface during photoelectrochemical water splitting — •waqas saddique, gerhard lilienkamp, and winfried daum — Institute of Energy Research and Physical Technologies, Technical University Clausthal, Clausthal-Zellerfeld, Germany

A detailed understanding of charge transfer across the electrode/electrolyte interface is required for the development of electrodes for efficient water splitting. We have studied the charge transfer processes across the n-GaP(100) photoanode/electrolyte interface at different photoelectrochemical (PEC) conditions. In a 0.02 M HCl electrolyte, high photoanodic currents from n-GaP(100) photoanodes related to photolytic water splitting were measured at low anodic potentials, these currents diminished at cathodic potentials as well as at high anodic potentials. Nyquist plots obtained from electrochemical impedance spectroscopy (EIS) results were analyzed with two different equivalent electrical circuits (EECs) for the electrode/electrolyte charge transfer pathways. For both EECs, the potential dependence of resistances and constant phase elements were determined from fits to Nyquist plots and then compared with the potential variation of the current in the cyclic voltammogram. XPS measurements revealed that the surface oxide consists mainly of Ga2O3, while small concentrations of GaPO4, P2O5 and metal-like Ga are also detected in the topmost layers. Our results suggest that energetically favorable absorption of hydroxide, persumably at metal-like surface Ga, and their subsequent oxidation at low anodic potentials lead to high currents.

O 70.4 Wed 15:45 MA 144

Epitaxial oxides as model electrodes for electrolyzer and fuel cell reactions at room temperature — •Marcel Risch, Julius Scholz, Janis Geppert, Lennart Köhler, Garlef Wartner, and Christian Jooss — Georg-August-Universität Göttingen, Institut für Materialphysik,

Energy carriers based on sustainable hydrogen are highly desirable for storage of intermittent renewable energy. The performance of the required electrolyzer and fuel cell technology could be improved significantly by a fundamental understanding of the basic reaction steps of the oxygen electrodes, which present the current bottleneck for electrocatalysis at room temperature. The chemistry and correlation physics of perovskite oxides can be tuned by chemical substitution to derive property-activity relationships [1]. Epitaxial thin films with optimized composition are very active for both the evolution as well as reduction of oxygen [2]. Moreover, perovskite oxide films of conductive (La,Sr)MnO3 showed terraces with unit cell step height and the perovskite structure was preserved after electrolysis in alkaline solution [3]. These properties make perovskite oxides ideal model surfaces to elucidate the catalytic mechanisms of oxygen evolution and reduction at room temperature. It will be discussed how the combination of materials physics, electrochemistry and spectroscopy leads to the desired mechanistic insight on selected perovskite oxides with defined surfaces.

References: [1] Risch et al., Catalysts 7, 139 (2017); [2] Risch et al., J. Am. Chem. Soc. 136, 5229 (2014); [3] Scholz et al., J. Phys. Chem. C 120, 27746 (2016), Scholz et al., Catalysts 7, 139 (2017).

O 70.5 Wed 16:00 MA 144

Operando Phonon Studies of the Protonation Mechanism in Highly Active Hydrogen Evolution Reaction Pentlandite Catalysts — •Ioannis Zegkinoglou[1], Ali Zendegani[2], Ilya Sinev[1], Ulf-Peter Apfel[3], Tilmann Hickel[2], and Beatriz Roldan Cuenya[1] — [1]Department of Physics, Ruhr-University Bochum, Germany — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [3]Inorganic Chemistry I, Ruhr-University Bochum, Germany

Synthetic pentlandite ($Fe_{4.5}Ni_{4.5}S_8$) is a promising electrocatalyst for hydrogen evolution, demonstrating high current densities, low overpotential, and remarkable stability in bulk form. The depletion of sulfur from the surface of this catalyst during the electrochemical reaction has been proposed to be beneficial for its catalytic performance. We have performed electrochemical operando studies of the vibrational dynamics of pentlandite under hydrogen evolution reaction conditions using ^{57}Fe nuclear resonant inelastic X-ray scattering [1]. Comparing the measured Fe partial vibrational density of states with DFT calculations, we have demonstrated that hydrogen atoms preferentially occupy substitutional positions replacing pre-existing sulfur vacancies. Once all vacancies are filled, the protonation proceeds interstitially, which slows down the reaction. Our results highlight the beneficial role of sulfur vacancies in the electrocatalytic performance of pentlandite and give insights into the hydrogen adsorption mechanism during the reaction. [1] I. Zegkinoglou et al., J. Am. Chem. Soc. 139, 14360 (2017).

O 71: Focus Session: Nanoscale Insights into Interfacial Electrochemistry II

Time: Wednesday 15:00–17:15 Location: HE 101

O 71.1 Wed 15:00 HE 101

From nanoparticle shapes to mechanisms: modeling the oxygen evolution reaction at IrO_2 nanoparticles from first-principles — •Daniel Opalka, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter — Technische Universität München

The efficiency and commercial viability of proton-exchange membrane (PEM) electrolysers depends critically on the anode catalyst. Chemical stability requirements currently limit the available catalyst materials to iridium oxide based materials. Experiments identified the surface morphology and associated iridium hydroxo groups as important factors in the oxygen evolution reaction mechanism, but the relevant structural features in operating PEM cells remain elusive. In this contribution we develop an ab initio thermodynamics based scheme to predict the surface stoichiometry and composition of individual IrO_2 facets as a function of the applied potential. Combined within a Wulff construction this yields the shape of IrO_2 nanoparticle catalysts at operating conditions. The determined potential-dependent transformations of surface hydroxo groups furthermore allow to conclude on Faradaic charge transfer processes as observed in cyclovoltammetric experiments. From this atomistic picture we finally derive a mechanistic model which explains important reaction steps in the water oxidation reaction.

O 71.2 Wed 15:15 HE 101

Selective solvent-induced stabilization of polar oxide surfaces in an electrochemical environment — •Su-Hyun Yoo, Mira Todorova, and Jörg Neugebauer — Department of Computational Materials Design, Max-Planck-Insitut fuer Eisenforschung GmbH, Duesseldorf, Germany

Solid/liquid interfaces are at the heart of many problems of practical importance, such as water electrolysis and batteries, photo catalytic water splitting, electro catalysis or corrosion. Understanding what surface structures form when the solid is immersed in an aqueous electrolyte is therefore of particularly high interest. Focusing on the ZnO(0001) surface as a typical example of a polar oxide surface, we study the thermodynamic stability of its surface reconstructions subject to the environmental conditions. We find that solvation effects are highly selective: They have little effect on surfaces showing a metallic character, but largely stabilize semiconducting structures, particularly those that have a high electrostatic penalty in vacuum. We will show that this selectivity has direct consequences for the surface phase diagram and discuss the mechanisms by which it is triggered.

[1] S.-H. Yoo, M. Todorova and J. Neugebauer (submitted)

Invited Talk O 71.3 Wed 15:30 HE 101

XPS of ionic liquids: from half-cell to in situ electrochemical measurements — •Annette Foelske-Schmitz[1], Markus Sauer[1], Daniel Weingarth[2], and Rüdiger Kötz[3] — [1]TU Wien, Vienna, Austria — [2]Heraeus Holding GmbH, Hanau, Germany — [3]Paul Scherrer Institut, Villigen, Switzerland

XPS is widely accepted to be a powerful tool to study electrochemically induced changes of the electrode/electrolyte interface. As electrochemical experiments are commonly performed under atmospheric pressure, XPS is usually not applied directly in the analyser chamber. Therefore, three experimental approaches may be distinguished: (i) ex situ, (ii) quasi in situ, and, (iii) in situ EC XPS [1]. The in situ approach may be realised using UHV compatible electrolytes such as ionic liquids (IL). IL are also known to provide large electrochemical stability windows making them attractive for certain electrochemical applications, such as double layer capacitors or lithium ion batteries. In this contribution quasi in situ [2] and in situ [3] EC XPS setups as well as half-cell measurements of IL [4] will be presented and discussed with respect to investigations of interfacial behaviour, stability windows, and interpretation of XPS data.

[1] A. Foelske-Schmitz, Ref. Mod. Chem., Mol. Sci. Chem. Eng., Elsevier, in press [2] A. Foelske-Schmitz, D. Weingarth, R. Kötz, Electrochim. Acta 56 1032 (2011)[3] D. Weingarth, A. Foelske-Schmitz, A. Wokaun, R. Kötz, Electrochem. Commun. 13 619 (2011)[4] A. Foelske-Schmitz, M. Sauer, JESRP, in press

15 min. break

Invited Talk O 71.4 Wed 16:15 HE 101

Single-Molecule Switching in 2D Materials at Solid-Liquid Interfaces — •Stijn F. L. Mertens — TU Wien, Institut für Angewandte Physik, 1040 Vienna, Austria

Living organisms are full of sophisticated molecular machines, and unravelling their structure and function continually inspires man-made nanotechnology, with expected applications from tribology to data storage.

In my talk, I will discuss mechanisms for controlled switching of the structure and properties of 2D materials at solid-liquid interfaces, from the collective scale down to single-molecule manipulation, at ambient temperatures and pressures. The 2D materials include self-assembled structures of tailored organic molecules but also hexagonal boron nitride, an atomically thin insulator. The switching events invariably depend on tipping the balance between intermolecular and adsorbate-substrate interactions, and may be controlled by a number of external stimuli: the interfacial potential at electrochemical solid-liquid interfaces, the chemical potential of ionic species in solution, intercalation of atomic species, or the electric field between an STM tip and the substrate.

References: Angew. Chem., Int. Ed. 53, 12951 (2014); Chem. Commun. 50, 10376 (2014); Small 1702379 (2017); Nature 534, 676 (2016)

O 71.5 Wed 16:45 HE 101

Electrochemical STM Imaging of J-Aggregates Immobilized on Au(111) — •Iris Dorner[1], Matthias Müllner[1], Ulrike Diebold[1], Jürgen Hauer[2], Graig N. Lincoln[3], and Stijn F.L. Mertens[1] — [1]TU Vienna, Institute of Applied Physics, Wiedner Hauptstr. 8-10/134, 1040 Vienna, Austria — [2]TU Munich, Associate Professorship of Dynamic Spectroscopy, Department of Chemistry, Lichtenbergstr. 4, 85748 Garching, Germany — [3]TU Vienna, Photonics Institute, Gusshausstr. 27, 1040 Vienna, Austria

J-aggregates are supramolecular assemblies of organic dye molecules with characteristic optical and exciton transport properties and have captured interest in photochemistry, photonics and materials science. Although widely characterized in spectroscopic experiments, models for their structure have been waiting for experimental evidence.

We present electrochemical scanning tunnelling microscopy studies with submolecular resolution of the J-aggregate-forming molecule 5,5',6,6'-tetrachloro-1,1',3,3'-tetraethylbenzimidacarbocyanine (TTBC). On bare Au(111), the molecules do not form an ordered structure, which we ascribe to kinetic trapping. If the gold substrate is modified by an iodide adlayer, favourable electrostatic interactions and enhanced lateral diffusion of TTBC yield long-range ordered structures that reflect the hexagonal symmetry of the substrate. Ongoing work aims to reveal to what extent the TTBC adlayer structure is representative of J-aggregates in solution.

O 71.6 Wed 17:00 HE 101

Nanoscale monitoring of temperature dependent lithium particle growth for solid state electrolytes — •Valon Lushta[1], Sebastian Badur[1], Dirk Dietzel[1], Bernhard Roling[2], and André Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig-University Gießen, D-35392 Gießen, Germany — [2]Department of Chemistry,Philipps-University of Marburg, D-35032 Marburg, Germany

Solid-state batteries are a promising approach to safer and more reliable electrochemical energy storage. However, compared to current liquid electrolytes these materials only show a low ion conductivity. In this context, understanding ion transport processes on the nanoscale is considered crucial for the development of improved solid electrolyte systems. Here we have employed a novel approach, where nanoscopic metallic lithium particles are deposited on a solid electrolyte surface by a biased AFM tip [1,2]. To verify, that quantitative values for the local ion mobility can indeed derived by this method, we have monitored the particle volume as a function of the sample temperature for the example of a Ohara lithium ion glass ceramic. From this data the Arrhenius activation energy for ion diffusion could then be calculated and was found to be in good accordance to macroscopic reference data. Additionally, we managed to perform high resolution mapping of the ion mobility by decreasing the particle volumes to only a few 10 nm^3.

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[1] S. Jesse et al., *Nano Lett. 11*, 4161-4167 (2011)

[2] J. Kruempelmann et al., *Electrochem. Comm. 18*, 74-77 (2012)

O 72: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 15:00–17:45 Location: HL 001

Invited Talk O 72.1 Wed 15:00 HL 001

Computational Approach to the Electronic Structure of Strongly Correlated Materials: Towards Theoretical Spectroscopy and Theory Assisted Material Design — •Gabriel Kotliar — Serin Physics Laboratory Rutgers University — Brookhaven National Laboratories

We will introduce a project, to build algorithms and a suite of open source codes, to compute the electronic structure of correlated materials. It involves different methods, to provide different compromises between speed and accuracy, and to treat different types of correlation (static and dynamic). The suite includes methods ranging from vertex corrected GW, rotationally invariant slave bosons and LDA+DMFT, and we will illustrate some of these methods (and their failures) in d and f electron systems.

O 72.2 Wed 15:30 HL 001

Spectral properties of Sr2IrO4 from first principles — •Cyril Martins[1], Benjamin Lenz[2], and Silke Biermann[2,3] — [1]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

The spin-orbit system Sr2IrO4 has raised tremendous interest recently, due to intriguing similarities to the high-Tc superconducting copper oxides.

We study the evolution of the electronic structure of Sr2IrO4 using a combination of ab-initio density functional theory and many-body techniques. The effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions are included on a first-principles level. We calculate the momentum-resolved spectral function and compare to recent photoemission data, finding good agreement with experiment.

O 72.3 Wed 15:45 HL 001

Role of non-local correlations in doped Sr_2IrO_4 — •Benjamin Lenz[1], Cyril Martins[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

When doping the spin-orbit system Sr_2IrO_4 recent photoemission experiments found pseudogap behavior at low temperatures, which raises the question of its relation to the pseudogap found in high-Tc superconducting copper oxides.

Here, we study the evolution of the electronic structure of Sr_2IrO_4 upon electron- and hole-doping by combining ab-initio density functional theory and two quantum cluster techniques. Our treatment includes the effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions on a first-principles level. We show that short-range antiferromagnetic fluctuations are crucial to account for the electronic properties of the material even in the high-temperature paramagnetic phase. Furthermore, pseudogap features in the momentum-resolved spectral function of the emerging exotic metallic state are analyzed and found to be in good agreement with experiment.

O 72.4 Wed 16:00 HL 001

Describing the coupled structural and metal-insulator transition in rare-earth nickelates with DFT+DMFT — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Perovskite rare-earth nickelates, $R\mathrm{NiO}_3$, display a rich phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT) that is accompanied by a structural distortion. This distortion breaks the symmetry between formerly equivalent Ni sites and is related to a charge disproportionation driven by correlation effects, resulting in an insulating state. Here, we employ density functional theory together with dynamical mean field theory (DFT+DMFT) to explore the interplay between lattice distortions and electronic correlation effects in these compounds. By utilizing a symmetry-based distortion mode analysis, we are able to isolate the specific lattice distortion occurring at the phase transition. Calculating total energies within DFT+DMFT then allows us to relax the structures with respect to this distortion. We find, that the resulting distortion amplitudes and its variation across the series are in good agreement with experimental results. Our work highlights the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom.

O 72.5 Wed 16:15 HL 001

Magnetocrystalline anisotropy of FePt: LDA+DMFT study — •saleem Ayaz Khan[1], Junqing Xu[2], johan Schott[3], Ondřej Šipr[1], and Jan Minár[1] — [1]University of West Bohemia, Pilsen, Czech Republic — [2]LMU Munich, Germany — [3]Uppsala University, Sweden

In our recent work (Phys. Rev B, 94, 144436, 2016) we employed ab initio methods (FLAPW and KKR) to get a reliable value for the magnetocrystalline anisotropy (MCA) energy of FePt. The theoretical MCA energy of FePt (3.0 meV) is significantly larger than the experimental value (1.3 meV), implying that the LDA cannot properly describe the MCA of FePt. Considering that the MCA essentially arises from spin orbit coupling it appears that to obtain reasonable agreement with experiments, it is necessary to include orbital correlations. To account realistically for both the electronic and geometric structure of materials, we use a combined density functional and dynamical mean field theory, LDA+DMFT. Our computation is based on the fluctuation exchange approximation and an analytic continuation method for the self-energy. Our results show that dynamical correlation effects are important for a correct treatment of the 3d-5d hybridization in FePt, which in turn plays a significant role for the magnetocrystalline anisotropy

O 72.6 Wed 16:30 HL 001

Diagnostics for plasmon satellites and Hubbard bands in transition metal oxides — •Steffen Backes[1], Hong Jiang[2], and Silke Biermann[1] — [1]Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau, France — [2]College of Chemistry and Molecular Engineering, Peking University, China

The generally accepted picture of $SrVO_3$ is that of a correlated electron metal where a renormalized quasi-particle peak at the Fermi level coexists with upper and lower Hubbard bands, separated by Coulomb interaction U. Recently, this picture has become blurred with the rise in interest in additional plasmonic satellites. Distinguishing plasmonic features from Hubbard bands is a non-trivial question. In this talk we employ combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") to discuss the processes that give rise to these different satellites and show how to identify their origin in realistic materials. We present an application of this scheme to different transition metal oxides, which we find to exhibit both Hubbard and plasmonic satellites at similar energetic positions.

O 72.7 Wed 16:45 HL 001

Phase transitions of the 2D Hubbard-Holstein model — •Teresa E. Reinhard[1], Uliana Mordovina[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In the 2d Hubbard-Holstein model at zero temperature, a quantum phase transition between Mott and Peierls insulator can be observed. Whether a metallic phase emerges in between remains an open question [1,2]. As the emergence of the Mott phase is a many body effect, a description beyond the mean field level is crucial. At the same time, a method that can cope with two dimensions is needed.

To address this open question, we have extended Density Matrix Embedding Theory (DMET) from the purely electronic case [3,4] to coupled fermion-boson systems. DMET is an embedding theory which benefits from the exponentially decaying correlation in most quantum systems thus allowing a description beyond mean field at low cost.

We show the phase diagram of the 2d Hubbard-Holstein model at zero temperature obtained for different cluster sizes. [1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012) [2] S. Wouters, C. A. Jiménez-Hoyos, G. K.-L. Chan, arXiv:1605.05547 (2016) [3] R. T. Clay and R. P. Hardikar, Phys. Rev. Lett 95, 096401 (2005) [4] J. Bauer, EPL 90 27002 (2010)

O 72.8 Wed 17:00 HL 001

A quantum embedding theory combining many-body perturbation theory with configuration interaction — •Marc Dvorak and Patrick Rinke — Department of Applied Physics, Aalto University School of Science, 00076-Aalto, Finland

We present a new quantum embedding theory called dynamical configuration interaction (DCI). It captures non-local and static correlation in an orbital active space with configuration interaction (CI) and high-energy, dynamic correlation in the complementary bath space with many-body perturbation theory (MBPT). The formulation is general, but we focus on molecular systems with an *ab-initio* Hamiltonian. The conceptual key to our approach is to replace the exact electronic Hamiltonian in the bath space with one of excitations defined over the correlated ground state. This transformation is naturally suited to the language and methodology of many-body Green's functions. Correlation in the bath is therefore described at the quasiparticle level with Green's functions instead of with the many-body wave function. Our approach avoids computational and conceptual difficulties associated with Green's function embedding and improves upon wave function methods by including dynamical correlation from the bath space. A major advantage to DCI is that it naturally treats ground and excited states on equal quantum mechanical levels. For ground state properties, we present dimer dissociation curves for H_2 and N_2 in excellent agreement with exact results. Excited states of N_2 give excellent agreement with experiment, and we demonstrate the scalability of our method by computing excited states of a free-base porphyrin molecule.

O 72.9 Wed 17:15 HL 001

Real-Structure Effects and Correlation in Layered Sodium Cobaltates — Sophie Chauvin[1,2], Silke Biermann[1], Lucia Reining[2], and •Claudia Rödl[3] — [1]Centre de Physique Théorique, École polytechnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire des Solides Irradiés, École polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Na-doped layered cobaltates Na_xCoO_2 feature a rich phase diagram with a plethora of physical phenomena ranging from metal-insulator transitions over magnetism to charge ordering. These instabilities of the electronic structure are mostly attributed to correlation effects within the quasi-2D CoO_2 layers. Here, we focus on $Na_{2/3}CoO_2$, a doping for which the system is metallic and exhibits an experimentally established charge disproportionation on the Co atoms.

We study the electronic properties of the CoO_2 layers and investigate the impact of the intercalated Na atoms on the electronic structure in the ordered layered superstructure. The problem is tackled from an *ab-initio* point of view using density-functional theory (DFT) and many-body perturbation theory (MBPT). Moreover, we study the static charge-density response of the material to understand instabilities in the system. Our approach complements recent model calculations from extended dynamical mean-field theory (EDMFT). The calculated results are compared to experimental spectroscopic data.

O 72.10 Wed 17:30 HL 001

Slave rotor approach to impurity models with correlated dp orbitals — •Jakob Steinbauer and Silke Biermann — École Polytechnique, Palaiseau, France

We propose a slave rotor method for the solution of many-orbital quantum impurity problems, which maps the original problem onto one with reduced degeneracy. This is particularly useful for the dynamical mean field theory treatment of transition metal oxides where the interactions between ligand states with d-electrons are all too often simply neglected. We derive a general formalism relying on an optimized effective model obtained from the variational principle of Feynman and Peierls and test the method in the atomic limit.

O 73: Surface dynamics: Reactions, elementary processes and phase transitions II

Time: Wednesday 16:45–18:00 Location: MA 043

O 73.1 Wed 16:45 MA 043

Near-Field Enhanced Photochemistry of Single Molecules in an STM Junction — •Hannes Böckmann[1], Sylwester Gawinkowski[2], Jacek Waluk[2], Markus B. Raschke[3], Martin Wolf[1], and Takashi Kumagai[1] — [1]Department of Physical Chemistry, FHI Berlin, Germany — [2]Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland — [3]Department of Physics, Department of Chemistry, University of Colorado, Boulder, USA

Optical near-field excitation of metallic nanostructures can be used to enhance photochemistry and promote photocatalysis. However, few studies have yet addressed near-field induced chemistry at the single-molecule level. Here we report the near-field enhanced tautomerization of porphycene on a Cu(111) surface in a scanning tunneling microscope (STM) junction. The light-induced tautomerization is mediated by photogenerated carriers in the Cu substrate. It is revealed that the reaction cross section is significantly enhanced in the presence of a Au tip compared to the far-field induced process. The strong enhancement occurs in the red and near-infrared spectral range for Au tips, whereas a W tip shows a much weaker enhancement, suggesting that excitation of the localized plasmon resonance contributes to the process. Additionally, the near-field enhanced tautomerization is examined in and out of the tunneling regime. Our results suggest that the enhancement is attributed to the increased carrier generation rate via decay of the excited near-field in the STM junction. Additionally, optically excited tunneling electrons also contribute to the process in the tunneling regime.

O 73.2 Wed 17:00 MA 043

Semiconductor surface chemistry induced by electronic excitation – tip-induced ether cleavage on Si(001) — Gerson Mette[1], Alexa Adamkiewicz[1], Tamam Bohamud[1], Marcel Reutzel[1], •Michael Dürr[2], and Ulrich Höfer[1] — [1]Philipps-Universität, 35037 Marburg — [2]Justus-Liebig-Universität Giessen, 35392 Giessen

Reactions of organic molecules on silicon typically proceed via an intermediate state and the conversion barrier between intermediate and final state determines the final products. Electronic excitation, e.g., by tunneling electrons from an STM tip, can open additional reaction channels which are not accessible by means of thermal activation.

Here we show that tip-induced cleavage of the datively bonded intermediate of THF on Si(001)[1] leads to covalently bound final configurations which are not observed for the thermally activated reaction. We find one single threshold in the dependence of the conversion rate on applied bias for all final configurations. Below the threshold, the conversion rate depends nonlinearly on the tunneling current, indicating a reaction induced via multiple excitations of vibrational modes.

Above the threshold, this dependence is linear, indicating direct excitation by electron transfer into the antibonding C-O orbital of THF. In the latter case, the molecules on the excited PES are not subject to the strong restrictions which control the transition state on the ground state PES, thus leading to the observed larger variety of final products. [1] G. Mette, et al., ChemPhysChem 15, 3725 (2014).

O 73.3 Wed 17:15 MA 043

Rotation and Translation of a Single Molecular Dipole — •Grant J. Simpson[1], Víctor García-López[2], James M. Tour[2], and Leonhard Grill[1] — [1]University of Graz, Graz, Austria — [2]Rice University, Texas, USA

Controlling matter on the atomic scale using the tip of a scanning tunneling microscope (STM) is now a well-established field. The *pushing* and *pulling* STM manipulations employ rather close-range interactions and can be used to position single atoms and molecules on a surface with exquisite precision. Furthermore, a number of molecular processes such as rotation and conformational switching can be induced through inelastic electron tunneling or through interaction with the electric field in the STM junction. Gaining control over the direction of rotation and translation of single molecules is more challenging though. In the current work it is shown that an in-built permanent molecular dipole can be used to achieve a high degree of control over the motion of a single molecule. Through interaction of this dipole with the electric field of the tip, unidirectional rotation and translation is demonstrated [1]. Additionally, by mapping the behavior of this motion, it is possible to visualize the internal electric dipole in a single molecule.

[1] G. J. Simpson, V. García-López, P. Petermeier, L. Grill, and J. M. Tour, Nat. Nanotechnol. 12 (2017) 604.

O 73.4 Wed 17:30 MA 043

O adatom diffusion in a dense CO matrix on Ru(0001) with video-rate variable temperature STM — •Ann-Kathrin Henss[1], Philipp Messer[1], Don C. Lamb[1], Rolf Schuster[2], and Joost Wintterlin[1] — [1]Chemie Department, Ludwig-Maximilians Universität München — [2]Institut für Physikalische Chemie, Karlsruher Institut für Technologie

To obtain reliable kinetic parameters of surface processes it is necessary to collect data over a wide range of temperatures. For scanning tunneling microscopes (STM) this range is usually limited by the slow imaging rates. We improved a home-built beetle-type STM by modifying the scan control unit and the data acquisition system to enable video-rate STM imaging with up to 50 images per second. The STM is also equipped with a liquid helium cryostat and heating facilities, giving access to temperatures between 50 and 500 K. The combination of temperature variability and video-rate imaging allows us to monitor surface diffusion of single atoms over a much broader temperature range than before. First experiments were performed on the diffusion of oxygen adatoms in a dense layer of CO molecules on Ru(0001). Videos of the moving oxygen atoms, obtained between -50 °C and room temperature and analyzed by particle tracking, show a surprisingly complex dynamic behavior. The data provide microscopic insight into atomic transport processes on "crowded surfaces", the typical situation in heterogeneous catalytic reactions.

O 73.5 Wed 17:45 MA 043

Phase Diagrams of Titanium Clusters in a Reactive Oxygen Atmosphere:a Replica-Exchange Grand-Canonical *ab initio* Molecular-Dynamics study — •yuanyuan zhou, matthias scheffler, and luca m. ghiringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft

TiO_2 has widespread applications such as photocatalysis, photovoltaics, and oxide electronics. To help elucidate the microscopic details of the catalytic processes, experimental and theoretical works have been performed on titanium-oxide clusters in the past decade (e.g., S. Bhattacharya *et al.*, PRB **91**, 241115 (2015)). Here, the replica-exchange (RE) grand-canonical (GC) molecular-dynamics method, recently developed by us, is used to explore $Ti_{4/8}$ cluster in contact with a reacting atmosphere of O_2 molecules. The method enables the unbiased, efficient calculation of complete $p-T$ phase diagrams. The system is modeled via DFT, at the PBE level. The GC ensemble is adopted to describe clusters in a reactive atmosphere. RE allows for an efficient sampling by shuttling configurations from regions of low T or high chemical potential (μ) to regions of high T or low μ. This massively parallel method requires no prior knowledge of the phase diagram and takes only the potential energy function together with the desired μ and T ranges as inputs. We identify the thermodynamically most stable phases of $Ti_{4/8}O_x$ at realistic T/p_{O_2} conditions, as a first step towards an understanding of the complex titanium-oxide surfaces at the atomistic level.

O 74: Nanostructures at surfaces: Other aspects

Time: Wednesday 16:45–18:30 Location: MA 141

O 74.1 Wed 16:45 MA 141

Asymmetric coupling on the chiral PdGa{111} surfaces — Samuel Stolz[1,2], Oliver Gröning[1], Harald Brune[2], and •Roland Widmer[1] — [1]Empa, nanotech@surfaces, 8600 Dübendorf, Switzerland — [2]EPFL, ICMP, 1015 Lausanne, Switzerland

Intermetallic PdGa exists in two enantiomeric crystal forms A and B due to its P213 space group and all its surfaces are chiral. Furthermore, the (111) and (-1-1-1) surface terminations of the same crystal form are structurally different. In particular, one is terminated by a single, isolated Pd atom (Pd1), while the other reveals isolated Pd trimers (Pd3). We demonstrated a 98% enantioselectivity of Pd1 and Pd3 by the adsorption of prochiral 9-Ethynylphenanthrene (9-EP) [1].

To profit from this high enantioselectivity we aimed to perform highly chiral asymmetric, covalent coupling reactions and have chosen an Azide-Alkine Huisgen Cycloaddition. Therefore, 9-EP as the alkine and 3-(4-Azidophenyl)propionic acid as the azide, were co-adsorbed on Pd1 and Pd3. The catalysed reaction is regiostereoselective on Pd1 and one out of four reaction products is favoured over the others yielding in an enantiomeric excess of up to 66%.

On the other hand, no reaction between 9-EP and the azide was observed on Pd3. Therefore, the reactivity for this particular reaction not only the depends on the d-band center, but much stronger on the surface geometry [2] as evidenced by the ensemble effect [1].

[1] J. Prinz, EPFL Thèse N°6337 (2014).

[2] J. K. Nørskov et al., Chem. Soc. Rev. 37 (2008) 2163-2171.

O 74.2 Wed 17:00 MA 141

Nanostructuring of dielectric surfaces by nanosecond laser irradiation — •Pierre Lorenz[1], Xiongtao Zhao[2], Martin Ehrhardt[1,2], Frank Frost[1], Joachim Zajadacz[1], Igor Zagoranskiy[1], Klaus Zimmer[1], and Bing Han[2] — [1]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, 04318 Leipzig, Germany — [2]Advanced Launching Co-innovation Center, Nanjing University of Science and Technology, 200 XiaoLingWei, 210094 Nanjing, Jiangsu, China

Nanostructuring of dielectric surfaces by nanosecond laser irradiationIndustrial utilisation of a laser-generated nano-structuring process requires a fast and cost-effective patterning approach. The so-called ISPM-LIFE (laser-induced front side etching using in-situ pre-structured metal layer) method allows the nanostructuring of dielectric surfaces in a two-step process: (i) a low laser fluence irradiation results in a nanopattern formation of the thin metal film, caused by laser-irradiation instabilities of the molten metal film and (ii) subsequent high-fluence laser pulses of those pre-structured metal pattern (e.g. holes in metal film, metal reticular-like structures and metal droplets) results in nanostructuring of the dielectric surface by *transferring* those metal patterns. The surface nanostructuring of fused silica and sapphire was studied with different nanosecond laser (wavelength 248 nm, 532 nm and 1064 nm using single and double laser pulses) and applying a thin metal layer (chromium and molybdenum with layer thicknesses from 10 nm to 50 nm). The intermediate and the final structures were investigated by AFM and SEM.

O 74.3 Wed 17:15 MA 141

Spin control induced by molecular charging in a transport junction — Sujoy Karan[1,2], •Carlos García[3], Michael Karolak[4], David Jacob[5,6], Nicolás Lorente[3,7], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [3]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, 20018 Donostia-San Sebastián, Spain — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [5]Departamento de Física de Materiales, Universidad del País Vasco, UPV/EHU, Av. Tolosa 72, 20018 San Sebastián, Spain — [6]IKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, 48013 Bilbao, Spain — [7]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Paseo Manuel de Lardizabal 5, 20018 Donostia-San Sebastián, Spain

We present experiments and calculations showing that the molecular electron affinity influences its spin transport. We use a scanning tunnelling microscope to trap a meso-substituted iron porphyrin, putting the iron centre in an environment that provides control of its charge and spin states. A large electron affinity of peripheral ligands is shown to enable switching of the molecular $S = 1$ ground state found at low electron density to $S = 1/2$ at high density, while lower affinity keeps the molecule inactive to spin-state transition. These results pave the way for spin control using chemical design and electrical means.

O 74.4 Wed 17:30 MA 141

Fabrication of micro-lenses on single-mode optical fibers by two-photon direct laser writing — •Sepideh Mazloomzadeh and Stefan Linden — Physics Institute, University of Bonn, D 53115

We report on the fabrication of different micro-lenses attached to the end facet of single-mode optical fibers using two-photon direct laser writing [1]. The lens types studied are plano-convex lenses and Fresnel lenses with diameters of several tens of microns. Such micro-lenses could be used in different applications such as laser to single mode fiber coupling or fiber to fiber coupling. We currently characterize the optical properties of the micro-lensed fibers and study the coupling efficiency and tilt effects.

[1] Timo Gissibl, Simon Thiele, Alois Herkommer & Harald Giessen, ”Sub-micrometre accurate free-form optics by three-dimensional printing on single-mode fibres”, Nat.Commun. 10,1038 (2016)

O 74.5 Wed 17:45 MA 141

Comparison of the switching behavior of 2D and 3D single molecules induced be mean of tip position and bias actions — •Loïc Mougel[1,2], Lukas Gerhard[1], Adam Gorczynski[1], Marcel Mayor[1,3], and Wulf Wulfhekel[1,2] — [1]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Physikaliches Institut, Karlsruhe Institute of Technology, 76131 Kasrlsruhe, Germany — [3]Department of Chemistry, University of Basel, St Johanns-Ring 19, 4056 Basel, Switzerland

Switching a molecule between different metastable states is interesting with regard to future applications in the field of molecular electronics.

We used scanning tunneling microscopy (STM) at temperature around 5K to study the switching behavior of individual tripodal organic molecules with a Tetraphanylmethane or a Triazine core within islands of different controlled order.

The molecules with different cores are three-dimensional or planar. They were deposited with a spraying and/or evaporation method on clean Au(111) surfaces. We were able to induce switching processes which allowed us to study the correlation of the switching behavior of neighboring molecules in threefold symmetric arrangement.

O 74.6 Wed 18:00 MA 141

Confined lattice dynamics in ultrathin Ge/Fe3Si/GaAs heterostructures — •Jochen Kalt[1,2], Małgorzata Sternik[3], Ilya Sergeev[4], Bernd Jenichen[5], Olaf Leupold[4], Ramu Pradip[1,2], Hans-Christian Wille[4], Przemysław Piekarz[3], Krzysztof Parlinski[3], Tilo Baumbach[1,2], and Svetoslav Stankov[1,2] — [1]1Laboratory for Applications of Synchrotron Radiation, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]2Institute for Photon Science and Synchrotron Radiation, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [3]Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland — [4]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [5]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

We studied the phonon properties of ultrathin ^{57}Fe$_3$Si layers in Ge/^{57}Fe$_3$Si/GaAs heterostructures as a model system for lattice dynamics modifications in metal/semiconductor interfaces. Epitaxial ^{57}Fe$_3$Si layers with thicknesses from 2ML to 36ML were grown on GaAs(001) substrates and capped by a 4 nm thick amorphous Ge layer. Sample characterization with various methods showed the formation of epitaxial Fe$_3$Si nanostructures with perfect stoichiometry and high interface quality. Nuclear Inelastic Scattering was used to determine the iron-partial phonon density of states at room temperature as a function of layer thickness. While the phonon DOS of the 36 ML sample is fully reproduced by the ab initio calculated DOS of bulk Fe$_3$Si, significant deviations are observed for lower interface thicknesses leading to anomalies in the thermoelastic properties.

O 74.7 Wed 18:15 MA 141

Nonlinear optical Circular Dichroism from plasmonic Metasurfaces — •Bernhard Reineke[1], Guixin Li[1], Shumei Chen[2], Franziska Zeuner[1], Martin Weismann[3], Ventsislav Kolev Valev[4], Kok Wai Cheah[5], Nicolae Panoiu[3], Shuang Zhang[2], and Thomas Zentgraf[1] — [1]Department of Physics, University of Paderborn, Warburger Straße 100 D-33098 Paderborn, Germany — [2]School of Physics & Astronomy, University of Birmingham, Birmingham B15 2TT, UK — [3]Department of Electronic and Electrical Engineering, University College London, Torrington Place, London, WC1 E7JE, UK — [4]Department of Physics, University of Bath, Claverton Down, Bath, BA2 7AY, UK — [5]Department of Physics, Hong Kong Baptist University, Kowloon Tong, Hong Kong

Circular Dichroism is the unequal absorption of left and right circularly polarized light. This effect is weak in planar Metasurfaces. Alternatively, Second Harmonic Generation Circular Dichroism (CD) from planar Metasurfaces is more responsive, than its linear analogue. We report a strong nonlinear circular dichroism for Second and Third Harmonic Generation from specially designed plasmonic Metasurfaces. In the future, these results, together with cheaper fabrication methods for Metamaterials enable a greater freedom in designing nonlinear optical devices.

O 75: Solid-liquid interfaces: Reactions and electrochemisty IV (joint session O/CPP)

Time: Wednesday 16:45–18:00 Location: MA 144

O 75.1 Wed 16:45 MA 144

Implicit solvation functionality for surface supercell calculations with the full-potential DFT code FHI-aims — •Jakob Timmermann, Marvin Lechner, Stefan Ringe, Harald Oberhofer, and Karsten Reuter — Technische Universität München

The necessity to account for solvation effects in electrochemical simulations is by now well established. Notwithstanding, explicitly resolving the solvation environment in first-principles based simulations leads to system sizes and sampling requirements that are still often computationally intractable. For this reason, implicit solvation methods, first pioneered over 80 years ago, are currently undergoing a renaissance. One such example is the modified Poisson-Boltzmann implicit solvation functionality that was recently implemented in the numeric atomic orbital based full-potential density-functional theory code FHI-aims [1]. Here, we extent this functionality to periodic boundary conditions, which allows to compute extended solid/liquid interfaces in supercell geometries. The performance and numerical efficiency of the approach is illustrated by computing the potential of zero charge for a range of reference close-packed metal surfaces.

[1] S. Ringe *et al.*, J. Chem. Theory Comput. 12, 4052 (2016).

O 75.2 Wed 17:00 MA 144

First-Principles Calculation of Solvent-Mediated Proton Transfer at the TiO$_2$(110) Surface: Kinetic Barriers and the Effect of Functionals — •Ahmad Agung, Thomas Stecher, Karsten Reuter, and Harald Oberhofer — Technische Universität München

To date, a majority of theoretical studies of (photo-)electrochemical surface reactions focuses on their thermodynamic feasibility. Only recently an ab initio molecular dyamics (AIMD) approach utilizing QM-MM embedding, explicit solvation and the HSE06 hybrid functional was applied to determine the kinetic barrier of H_2O dissociation on a rutile $TiO_2(110)$ surface [1]. Despite advanced sampling techniques and a comparatively small QM region, the use of the hybrid functional rendered these simulations computationally extremely expensive. To this end, we assess in how much generalized-gradient approximation (GGA) functionals can be employed to reduce the computational cost. Not too surprisingly, we find the inferior GGA energetics to yield a significantly different reaction barrier, when directly evaluating GGA-based AIMD trajectories. We therefore assess in how much these GGA trajectories yield at least an appropriate sampling of phase space, thereby offering computational savings by restricting the expensive hybrid level calculations to snapshots along these trajectories.

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

O 75.3 Wed 17:15 MA 144

Beyond Catalyst Screening for Electrocatalytic Materials – Importance of Active Site Structure, Mechanism, and Kinetics for the OER on Transition Metal Oxides — •Craig Plaisance, Simeon Beinlich, and Karsten Reuter — Technische Universität München, Germany

Over the past decade or so, the computational design of catalysts for electrochemical reactions has been dominated by an approach in which the catalytic performance of a material is quickly estimated by calculating the values of one or two atomic-level descriptors, typically binding energies of key intermediates on a low index surface of the material. While this approach allows for rapid screening of a vast number of catalyst materials and has indeed identified improved catalysts in several cases, it is based on rather drastic assumptions and can thus only give a rough estimate of catalytic performance. This talk examines the suitability of the descriptor-based screening approach for the OER on doped 3d transition metal oxides, a promising class of earth-abundant materials for catalyzing this reaction. Specifically, we examine whether or not the scaling and Bronsted-Evans-Polanyi relations on which the screening approach is based are robust with respect to changes in the geometry of the active site and the mechanism. We also address whether or not it is necessary to consider the kinetics of certain reaction steps in addition to the thermodynamics. In the end, we conclude that perhaps a more detailed understanding of the quantum chemical properties controlling electrocatalytic performance is needed in order to rationally design an optimal active site.

O 75.4 Wed 17:30 MA 144

Band alignment at semiconductor/water interfaces using explicit and implicit descriptions for liquid water — •Nicolas Hörmann[1], Zhendong Guo[2], Francesco Ambrosio[2], Oliviero Andreussi[1], Alfredo Pasquarello[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS) and MARVEL, EPFL, Lausanne, Switzerland — [2]Chair of Atomic Scale Simulations (CSEA) and MARVEL, EPFL, Lausanne, Switzerland

We compare the band alignment of several semiconductor/water interfaces for GaAs, GaP, CdS and TiO2 as determined from explicit water ab-initio molecular dynamics simulations based on density functional theory (DFT) to results obtained within a DFT + implicit solvation model (SCCS) [1] as implemented in ENVIRON. It has been demonstrated that solvation effects are an important ingredient to describe the interface energetics in electrochemical systems adequately [2,3], however, it is still unclear how the choice of the explicit water molecules included affects the computational results. This work will allow us to estimate the expected errors of using implicit solvation models, with and without thermodynamic sampling and can serve as a guideline for the amount of interfacial water that should be treated quantum mechanically. [1] O. Andreussi, et al., J. Chem. Phys. 136, 064102 (2012); [2] L. Sementa, et al., Catal. Sci. Technol., 6, 6901-6909 (2016); [3] J. Huang , N. Hörmann, et al. submitted to Nature Materials (2017), under review

O 75.5 Wed 17:45 MA 144

On the enhanced self-dissociation of water by bidimensional nanoconfinement — •Daniel Muñoz-Santiburcio[1,2] and Dominik Marx[2] — [1]CIC nanoGUNE, Tolosa Hiribidea 76, 20018 San Sebastián, Spain — [2]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

Nanoconfined liquids present strikingly different properties compared to the bulk regime. Water in particular is the subject of intense investigation, and in previous works we described how nanoconfinement affects the mechanisms and energetics of chemical reactions therein [1] and also the peculiar differences between the structural diffusion mechanism of H^+(aq) and OH^-(aq) compared to the bulk [2,3]. Now, we present interesting results of advanced *ab initio* simulations which show how bidimensional nanoconfinement enhances one of the most important reactions in water, namely the self-dissociation of H_2O(aq) into H^+(aq) and OH^-(aq) [4]. This surprising feature goes hand in hand with the enhancement of the parallel component of the dielectric constant tensor of the nanoconfined water layer.

[1] D. Muñoz-Santiburcio and D. Marx, *Chem. Sci.* 8 (5), 3444-3452 (2017).

[2] D. Muñoz-Santiburcio and D. Marx, *Nat. Commun.* 7, 12625 (2016)

[3] D. Muñoz-Santiburcio, C. Wittekindt and D. Marx, *Nat. Commun.* 4, 2349 (2013)

[4] D. Muñoz-Santiburcio and D. Marx, *Phys. Rev. Lett.* 119, 056002 (2017).

O 76: Ultrafast Electron and spin dynamics at interfaces III

Time: Wednesday 17:30–18:30 Location: MA 005

O 76.1 Wed 17:30 MA 005

Coherent many-particle excitations in NiO ultrathin films — •Konrad Gillmeister[1] and Wolf Widdra[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

Strong electronic correlation in NiO causes the appearance of a charge-transfer gap (CTG). Its lower and upper edges (Hubbard bands) are formed by Ni 3*d* electrons. In this contribution we focus on the electron dynamics after exciting electrons into the upper Hubbard band.

Using time-resolved two-photon photoemission spectroscopy (2PPE) on 1–20 monolayers (ML) NiO ultrathin films on Ag(001) we find that electrons decay within 15 fs across the CTG. However, there is a second long-living contribution to the 2PPE signal which is thickness- and temperature-dependent: periodic intensity modulations in the detected time-resolved signal near the vacuum cut-off with a lifetime of ∼350 fs are found for NiO film thicknesses beyond 5 ML and temperatures below 470 K for 10 ML (560 K for 20 ML). These oscillations are exlained by intra-gap states which are indirectly but coherently addressed by an instantaneous decay of excited electrons and which are subsequently probed. A simultaneous excitation of magnons is also discussed.

O 76.2 Wed 17:45 MA 005

Time-resolved photoelectron spectroscopy with high-order harmonics: Surface photovoltage shift at $SiO_2/Si(001)$ interfaces with nonlinear optical excitations — •Robin Kamrla[1,2], Cheng-Tien Chiang[1,2], Andreas Trützschler[1,2], Michael Huth[2], Frank Oliver Schumann[2], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

We investigate the fluence and doping dependence of surface photovoltage shifts (SPV) at $SiO_2/Si(001)$ interfaces. Charge carriers are excited by 300 fs laser pulses at repetition rates of 0.2 to 0.7 MHz with photon energies of $h\nu_{pump} = 1.2$ or 2.4 eV, and subsequently probed by high-order harmonics with $h\nu_{probe} = 22.6$ eV. On SiO_2/p-Si(001) we observe a SPV of 250 meV upon excitation with $h\nu_{pump} = 1.2$ eV towards higher energies, whereas on SiO_2/n-Si(001) the SPV reverses its sign and has a smaller magnitude of 140 meV. Upon excitation with $h\nu_{pump} = 2.4$ eV a maximum SPV at SiO_2/p-Si(001) of 350 meV is observed. Moreover, SPV at SiO_2/p-Si(001) shows a nonlinear fluence dependence at $h\nu_{pump} = 1.2\,\text{eV}$, which significantly differs from that of $h\nu_{pump} = 2.4\,\text{eV}$. In this talk the dynamics of SPV as well as its fluence dependence will be discussed.

O 76.3 Wed 18:00 MA 005

The one-step model of 2PPE in its layer-KKR formulation — •Jürgen Braun and Hubert Ebert — Dept. Chemie, LMU München, Germany

Recently a theoretical frame for the description of two-photon photoemission has been developed by the authors. 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 pump pulse that drives a system out of equilibrium [1]. The fully relativistic formalism has now been generalized to angular resolution in both the initial and intermediate state by means of layer-KKR multiple scattering techniques. First examples of angular-resolved 2PPE calculations on Fe(100) will be presented. Furthermore, correlation effects will be accounted for in this spectroscopical study by means of a static self-energy $\Sigma^{DMFT}(E)$ obtained for Fe from dynamical mean-field theory.

[1] J. Braun, R. Rausch, M. Potthoff , and H. Ebert, One-step theory of two-photon photoemission, Phys. Rev. B **94**, 125128 (2016)

O 76.4 Wed 18:15 MA 005

Asymmetric electron and hole dynamics in the Rashba material BiTeI — •Sophia Ketterl[1], Marco Polverigiani[1], Vladimir Voroshnin[2], Beatrice Andres[1], Alexander Shikin[2], and Martin Weinelt[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]St. Petersburg State University, Institute of Physics, Uljanovskaya 1, 198504 St. Petersburg, Russia

Due to strong spin-orbit coupling and non-centrosymmetric crystal structure, the narrow band-gap semiconductor BiTeI hosts Rashba-split surface and bulk bands. This makes BiTeI a promising material for the generation of spin-polarized currents. It is intrinsically n-doped and exhibits additional strong band-bending at its polar surfaces, leading to partially occupied electron- and hole-like surface states for Te and I termination, respectively.

We studied the elecron and hole dynamics in the suface state and bulk conduction band on the Te-surface with time-resolved ARPES and observed a strong asymmetry for carriers close to the Fermi level. Electrons behave according to Fermi-liquid theory, while hole lifetimes decrease towards E_F. We attribute this behavior to drift currents due to the surface band bending and the influence of a plasmon decay channel as predicted by Eremeev *et al.* in *JETP Lett.* **96**, 437 (2012).

O 77: Poster: Plasmonics and Nanooptics

Time: Wednesday 18:15–20:30 Location: Poster A

O 77.1 Wed 18:15 Poster A

Spectroscopic investigation of periodic plasmonic superstructures — •Ekaterina Ponomareva and Matthias Karg — Heinrich-Heine-University Düsseldorf, Physical Chemistry I, Düsseldorf, Germany

Nanoparticles with a plasmonic metal core and a soft cross-linked hydrogel shell spontaneously self-assemble at an air/liquid interface forming periodic monolayers [1]. These layers can be transferred on glass substrates yielding substrate-supported superstructures with hexagonally arranged plasmonic nanoparticles at inter-particle distances of a few hundred nm. Due to the spatial proximity and the periodicity of the array, localized surface plasmons of metal cores can couple to diffractive modes and thus support surface lattice plasmon resonances [2]. By embedding the monolayer into a gain-medium these resonances can be enhanced.

Here we will demonstrate the angular-dependent optical behavior of periodic plasmonic monolayers. UV-vis measurements show different optical properties for dilute particles in aqueous dispersion, the assembled monolayers and the monolayers upon embedding in a gain matrix. A home-made lasing-spectrometer was used to investigate the collective optical response of the plasmonic lattices in dependence on the detection and incident angle. With the set-up it is possible to observe the near-field and radiative plasmonic coupling effects in colloidal monolayers.

[1] K. Volk et al., Adv. Mater. 24 (2015), 7332

[2] K. Volk et al., Adv. Optical Mater. 5 (2017), 1600971

O 77.2 Wed 18:15 Poster A

Development of an optical near-field microscope — •hamed abbasi[1,2], igor shavrin[1], and klas lindfors[1] — [1]University of Cologne, Department of Chemistry, Cologne, Germany — [2]University of Bonn (Bonn-Cologne Graduate School for Physics and Astrophysics), Bonn, Germany

Scanning near-field microscopy is an outstanding method to investigate the features of materials on the deeply subwavelength scale. We develop and characterize a probe consisting a single gold nanoparticle for scanning near-field optical microscopy. The tip-particle system is locked to the surface within a distance of a few nanometers. After locking the distance, the surface can be scanned by using a 3-D Piezo stage to locally enhance light-matter interactions.

O 77.3 Wed 18:15 Poster A

Plasmonic fluorescence enhancement in cyanobacterial Photosystem I — •Daniel Fersch[1], Sebastian Pres[1], Bernhard Huber[1], Viktor Lisinetskii[1], Heiko Lokstein[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Chemical Physics and Optics, Charles University Prague, 121 16 Praha 2, Czech Republic

We investigate plasmon-enhanced fluorescence in thin films of Photosystem I (PS I) spin-coated with Au nanorods. Single hot spots attributed to the plasmonic fluorescence enhancement were observed by laser-scanning fluorescence microscopy. The extremely weak fluorescence signal of PS I excited by a HeNe laser is filtered by lock-in amplification.

The role of PS I is light-induced electron donation, so an interesting question is whether plasmonic interaction has an effect on the rate of charge separation, and thus photoelectron emission. To measure this we plan to extract the electrons from the PS I using photoemission electron microscopy. Finally, we intend to combine this method with ultrafast multidimensional spectroscopy to track transfer dynamics in space and time [1].

[1] M. Aeschlimann et al., Science 333, 1723 (2011)

O 77.4 Wed 18:15 Poster A

Plasmonic cavities and resonators in crystalline particles: fabrication and optical properties — •Manuel Gonçalves[1], Amos Kiyumbi[1], Joseph Iduwe[1], Frederike Erb[1], Gregor Neusser[2], Christine Kranz[2], Othmar Marti[1], and Kay Gottschalk[1] — [1]Ulm University - Institute of Experimental Physics, Ulm, Germany — [2]Ulm University - Institute of Analytical and Bioanalytical Chemistry, Ulm, Germany

Crystalline particles of gold and silver offer the best quality for the fabrication of plasmonic cavities, milled by focused ion beam (FIB). Due to the smoothness of the metal surface and consequent low absorption and radiation losses, groove cavities and other resonators can strongly enhance the near-fields and reach large Purcell factors. We have investigated theoretically and experimentally the reflection spectra of arrays of cavities milled in gold and silver particles and the fluorescence of dye molecules localized near silver particles. Metasurfaces formed by arrays of cavities may work as a band selective absorbing filter, or as a polarizer. Moreover, we have found that the sharp edges of the silver particles strongly enhance the dye fluorescence.

O 77.5 Wed 18:15 Poster A

STM-based time domain analysis of exciton generation in thin C_{60} films in the limit of single charge injection. — •Anna Rosławska[1], Pablo Merino[1], Christoph Grosse[1,2], Christopher Leon[1], Markus Etzkorn[1], Klaus Kuhnke[1], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]NanoPhotonics Centre, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [3]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The performance of organic light emitting diodes is controlled by charge and exciton dynamics which can be probed by time-resolved spectroscopies. Many methods, however, are sensitive only to mesoscopic transport properties for large charge density distributions. Here, we explore locally the single charge and single exciton regime using time-resolved scanning tunneling microscope-induced luminescence (TR-STML). We study excitonic emission centers (ECs) in a model system of C_{60} thin films on Au(111). ECs exhibit single photon emission due to single exciton trapping near structural defects. We apply 100 ns voltage pulses to turn the photon emission from the EC on and off and record time-resolved electroluminescence as a function of tip-sample distance. The observed dynamics is due to single electron and single hole injection and can be analyzed by employing a kinetic model which perfectly fits the recorded transients. The electric field dependence of the obtained time constants allows characterizing the energy barrier for electron injection at the C_{60} - Au(111) interface.

O 77.6 Wed 18:15 Poster A

Circular dichroism calculation of plasmonic nanohelices by boundary element method — •Daniel Nürenberg and Helmut Zacharias — Physikalisches Institut & Center For Soft Nanoscience, Münster, Germany

We present calculations on absorption, scattering and near-fields of plasmonic Ag, Cu and Ag:Cu alloy nanohelices from the UV to the near infrared of the optical spectrum. The calculations were carried out with a boundary element approach using the MNPBEM toolbox [1]. The inherent chirality of the nanohelices leads to a strong circular dichroism (CD). Furthermore we study the CD regarding different geometries, i.e. the size of the nanohelices in pitch and length around 100 nm. We compare the results for free helices and for helices attached to a silicon substrate and find for both very similar distributions of the intensities on the surface of the particles. The simulations can be compared with experimental reflectivity measurements.

[1] J. Waxenegger, A. Trügler, and U. Hohenester, Comput. Phys. Commun. 193, 138 (2015).

O 77.7 Wed 18:15 Poster A

Shaping Femtosecond Laser Pulses for Plasmonics — •Christoph Schnupfhagn, Moritz Heindl, Jonas Albert, and Markus Lippitz — Experimental Physics III, University of Bayreuth, Germany

Pulse shapers allow to modify phase and amplitude of ultrafast laser pulses in an almost arbitrary manner. This is especially favourable for nonlinear spectroscopy as electric fields for multiphoton processes can be precisely engineered. Combined with plasmonic nanostructures the optical near field can be controlled in space and time. In our experiment, we use a liquid crystal based spatial light modulator to reshape 8fs laser pulses in frequency space. The challenge is to couple the pulses into a high NA microscope without significant broadening in time domain. Here we present our experimental setup for pulse compression in the focal plane. Moreover, we give an overview how the spatiotemporal control of optical fields can be utilized in future experiments.

O 77.8 Wed 18:15 Poster A

Simulation of plasmonic nanoantennas excited by orbital angular momentum light — •Richard M. Kerber[1,2], Jamie M. Fitzgerald[2], Sang Soon Oh[2,3], Ortwin Hess[2], and Doris E. Reiter[1,2] — [1]Institut für Festkörpertheorie, Universität Münster, 48149 Münster, Germany — [2]Department of Physics, Imperial College London, London SW7 2AZ, United Kingdom — [3]School of Physics and Astronomy, Cardiff University, Cardiff CF24 3AA, United Kingdom

Orbital angular momentum light beams offer the possibility to encode additional information in the phase of the light beam, which makes them attractive for future communication technology. Here we study the interaction of orbital angular momentum light with plasmonic nanostructures and analyse the excited modes. Based on three different numerical and analytical methods, we show that for various combinations of polarization and orbital angular momentum of the incident light beam the scattering cross-section of rotation-symmetrical nanorod antennas displays different resonance modes [1]. The modes can be classified into bright and dark modes with their own resonance wavelengths. We compare the simulation results of the boundary element method with finite-difference time-domain simulations. Additionally we compare the numerical results with our analytical line antenna model. We discuss advantages and disadvantages of the three different approaches. [1] Kerber et al., ACS Photonics, 4, 891-896 (2017)

O 77.9 Wed 18:15 Poster A

Spatial and temporal separation of plasmon-induced hot carriers by time- and energy-resolved PEEM — •Michael Hartelt[1], Anna-Katharina Mahro[1], Tobias Eul[1], Benjamin Frisch[1], Eva Prinz[1], Deirdre Kilbane[1,2], Benjamin Stadtmüller[1], Mirko Cinchetti[1,3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]School of Physics, University College Dublin, Ireland — [3]Experimentelle Physik VI, Fakultät Physik, TU Dortmund, Germany

The generation of hot carriers through the internal decay of plasmons in metallic materials has received considerable attention lately, due to its wide range of potential applications [1]. Understanding the differences between photo-induced and plasmon-induced hot electrons is essential for the construction of devices for plasmonic energy conversion. We use a two-color femtosecond pump-probe scheme in time-resolved 2-photon-photoemission (TR-2PPE) to address the population dynamics of excited electrons in metals. We are able to separate the spectroscopic signature of the pure plasmon-induced hot carriers from that of directly photo-excited carriers by following the spatial evolution of photoemitted electrons with energy-resolved Photoemission Electron Microscopy (PEEM) during the propagation of a Surface Plasmon Polariton (SPP) along an Au surface. This allows us to study plasmon-induced hot carrier dynamics on the femtosecond and nanometer scale.

[1] Brongersma et al., Nature nanotechnology 10.1 (2015)

O 77.10 Wed 18:15 Poster A

Ellipsometric investigation of the interaction of surface and localized plasmons and registration of their splitting — •Eugene Bortchagovsky — Institute of Semiconductor Physics of NAS of Ukraine, pr. Nauki 41, Kyiv 03028, Ukraine

Two interacting resonances can hybridize and split with energy gap between two hybridized dispersion curves instead of their intersection. We used ellipsometry to investigate the interaction of surface plasmon with localized resonances of nanoparticles deposited on the surface.

Ellipspmetric measurements were made as in the standard configuration with external reflection as in the Kretschmann geometry with internal reflection. Spherical gold particles from "Nanopartz" were deposited from solution on gold films with the thickness of about 40nm deposited on BK-7 slides. For measurements in Kretschmann geometry slides were attached to BK-7 rectangular prism by matching index liquid from "Cargil". Dispersion curves were restored from the position of dips in measured ellipsometric spectra of "psi" angle for the system with nanoparticles with the diameter of 50nm.

Presented results clearly demonstrate existence of few plasmon resonances localized on nanoparticles. The third resonance may be multipolar in addition to two (longitudinal and transverse) dipolar ones lifting of the degeneration of which is produced by the interaction with surface. All localized resonances hybridize with the surface plasmon producing splitting instead of the crossing of initial dispersion dependences. Parts of dispersion curves obtained at external and internal reflection join each other.

O 77.11 Wed 18:15 Poster A

Grating Coupling to Surface Phonon Polaritons with an Infrared Free-Electron Laser — •Marcel Kohlmann, Nikolai C. Passler, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der Max-Planck-Gesellschaft

When coupling infrared electromagnetic waves and optical phonons at the surface of a polar dielectric material, surface phonon polaritons (SPhPs) can be created within the Reststrahlen band between transversal and longitudinal optical phonons. SPhPs have a longer lifetime than surface plasmon polaritons (SPPs) which makes them promising candidates to overcome the loss problems assocciated with the short life times of SPPs. Since surface polaritons are non-radiative large momentum states, they cannot be excited from free space, but instead require nanostructures[1], prisms[2] or gratings[3] to provide the extra momentum.

Here we use gratings etched into a SiC surface to excite propagating SPhPs with a infrared free electron laser. Reflectance measurements are employed to optimize the SPhP excitation efficiency of the grating structures. Finally, we probe the resonant light emission from a second grating of different period of well-defined distance from the first grating to investigate the propagation of the SPhPs at a flat surface.

[1] Razdolski et al., Nano Lett. 16, 6954 (2016)
[2] Passler et al., ACS Photonics 4, 1048 (2017)
[3] Hafeli et al., J. Appl. Phys. 110, 043517 (2011)

O 77.12 Wed 18:15 Poster A

Imaging of near fields on nanoscopic scale by using Atomic Force Microscopy (AFM) — •Christoph Bauschke, Kai Wardelmann, Sven Kraft, Ingo Barke, and Sylvia Speller — University of Rostock, Institute of Physics, 18059 Rostock, Germany

The optical tweezers phenomenon illustrates, that light is applying an optically induced forces while interacting with matter [1]. Our aim is the determination of optically induced forces by using Atomic Force Microscopy and illumination of metal nanostructures by time-modulated light. A lock-in amplifier serves to determine the share of the cantilever deflection, induced by light. On triangular islands of Au an optically induced effect on the cantilever deflection appears to be present, however this contrast is neither depending on the shape nor fully vanishing during dark phases suggesting other effects being involved. Improvements with respect to embedding of the metal nanostructures, better resonance between laser light and plasmon frequency of nanopartciles, and using more appropriate modulation frequencies are applied. Respective deflection maps could reveal dedicated light-induced features.

[1] Maragò et al., Nature Nanotechnology 8, (2013)

O 77.13 Wed 18:15 Poster A

Theory of coherent energy transfer between molecular exciton and gap plasmon induced by a scanning tunneling microscope — Lei-Lei Nian and •Jing-Tao Lü — School of Physics and Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, 430074 Wuhan, P. R. China

The coupling between molecular exciton and gap plasmons plays a key role in single molecular electroluminescence induced by a scanning tunneling microscope(STM). But it has been difficult to clarify the complex experimental phenomena. By employing the nonequilibrium Green's function technique, we propose a general theoretical approach to understand the light emission from single molecule and gap plasmons near a metal surface excited by the tunneling current. It is shown that the coherent energy transfer between the gap plasmon and molecular exciton leads to a significant Fano resonance when the molecule is located in the proximity of the STM tip. Different line shapes have been observed in recent experiemnts. Being applied to these experiments, our theory can provide a consistent and quantitative account of the experimental results from an energy transport point of view. This theoretical approach allows one to explain and predict the complex energy transfer processes, such as field-matter interaction and quantum interference, important for the further development in this field.

O 77.14 Wed 18:15 Poster A

Density matrix formalism in ultrafast electron microscopy — •Sergey V. Yalunin, Katharina E. Priebe, and Claus Ropers — University of Göttingen, 4th Physical Institute, Göttingen 37077, Germany

Electron-photon interactions are currently a subject of high interest in ultrafast electron imaging and microscopy [1]. Beyond the use in optical near-field imaging, such interactions may be important for the observation of quantum entanglement dynamics in solids, in the context of pump-probe experiments, using the free single-electron state as a quantum probe. However, this requires both a proper theoretical description of the underlying quantum processes and a quantum reconstruction algorithm of the electron state. Due to the limited number of projective measurements, the quantum reconstruction becomes essentially ill-posed in the sense that the matrix transformation describing the measurement does not have a bounded inverse. To demonstrate the feasibility of quantum reconstruction, we consider a situation where electrons initially prepared in a pure quantum state interact with two partially coherent laser pulses focused on a nanostructure. We reconstruct the final mixed quantum state of the electron ensemble and the properties of the laser field, contrasting the results with recent data [2] obtained with the Göttingen Ultrafast Transmission Electron Microscope (UTEM).

[1] B. Barwick, and A. H. Zewail, Nature 462, 902-906 (2009).
[2] K. E. Priebe et al., Nature Photonics 11, 793-797 (2017).

O 77.15 Wed 18:15 Poster A

Simulations of the magneto-plasmonic response of hybrid Bi-YIG/Au nanostructures — •Philipp Lang, Spiridon D. Pappas, and Evangelos Th. Papaioannou — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, Germany

The strong localization of light, which can be induced by surface plasmons, enhances the magneto-optical response of ferromagnetic materials [1]. In this work, we simulated the magneto-optical response of bismuth substituted yttrium iron garnet (Bi-YIG) thin films containing gold nanoparticles (AuNPs) with the aid of the simulation Software CST STUDIO. Specifically, the longitudinal magneto-optical Kerr effect (L-MOKE) has been simulated from the orthogonal components of the radiated electric field in the far field region and the results have been compared with the experimental. In order to explain the trend of the anomalous Kerr effect, which is attributed to the localization of the electric field by the AuNPs, the Near Field enhancement has been calculated and correlated to the Far Field results. The Near and Far field simulations have been performed by using unit cell boundary conditions for different angles, as well as for different wavelengths of the incident light.

[1] M. Rollinger et al., Nano Lett. 16, 2432 (2016).

O 77.16 Wed 18:15 Poster A

Scanning near-field optical spectroscopy with an inline interferometer for probing local absorption — •Jens Brauer, Jinxin Zhan, Petra Gross, Manuela Schiek, and Christoph Lienau — Carl von Ossietzky Universität Oldenburg

Combining spectroscopy methods with nanoscale probing techniques such as scanning near-field optical microscopy (SNOM) helps to measure vibrational fingerprints, quantifiy chemical composition or study the interaction of light with plasmonic nanoparticles or hybrid nano structures. Until now local spectra on the nanoscale are mainly measured indirectly, for example by repeated SNOM scans using monochromatic light and tuning the wavelength of the laser or by Fourier transform interferometry techniques. Nanoscale spectroscopy with SNOM is thus limited either in spectral resolution or in scan speed. A direct spectrometer approach is usually thought not to be possible since high-frequency modulation techniques are needed for background suppression.

We demonstrate a way to suppress background fields over a broad spectral range employing an inherently stable in-line interferometer in a homodyne detection scheme. In combination with a fast line camera it allows to directly acquire spectra employing existing modulation techniques. We record near-field spectra with a spatial resolution of 20 nm and reveal a spectral variation below the resolution limit of wide-field microscopy. With a microscopic model of the sample we relate this spectral variation to a local change of the morphology.

O 77.17 Wed 18:15 Poster A

Light trapping and localization in a-Si:H absorber layers with tailored nanotextures — Martin Aeschlimann[1], Felix Becker[2], Tobias Brixner[3], •Benjamin Frisch[1], Michael Hartelt[1], Matthias Hensen[3], Thomas H Loeber[4], Walter Pfeiffer[2], Sebastian Pres[3], Bernd Stannowski[5], and Helmut Stiebig[2] — [1]Fachbereich Physik and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern — [2]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld — [3]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [4]Nano-Structuring-Center, Erwin-Schrödinger-Str. 13, 67663 Kaiserslautern — [5]Helmholtz-Zentrum Berlin, PVcomB, Schwarzschildstr. 3, 12489 Berlin

The enhanced absorbtion for near-IR wavelengths in hydrogenated amorphous silicon (a-Si:H) thin films deposited on a nanotextured zinc oxide (ZnO) surface has been attributed to thermionic emission caused by Anderson localization of light [1]. FDTD simulations reveal that light localization only occurs for distinct spatial frequency ranges of surface roughness. Here a focused ion beam based fabrication technique is applied to tailor the ZnO towards a disordered system with enhanced absorption. The actual light trapping and absorption is investigated using time- and energy-resolved electron emission microscopy. We observe localized modes and high nonlinearities supporting the theory of thermionic emission after excitation with fs-pulses of 800 nm wavelength. [1] Nature Photonics 9, 663-668 (2015)

O 77.18 Wed 18:15 Poster A

Three-dimensional plasmonic nanostructure design for boosting photoelectrochemical Activity — •rui xu, liaoyong wen, zhijie wang, huaping zhao, shipu xu, yan mi, yang xu, max sommerfeld, yaoguo fang, and yong lei — Am Ehrenberg 2, 98693 ilmenau

An innovative approach is presented to construct three-dimensional pillar/truncated-pyramid (PTP) plasmonic nanostructure arrays. A CdS film on the Au PTP demonstrates the advantage of PTP plasmonic structures for light trapping, leading to about 3 and 2 times enhancement photocurrent density at -0.4 V vs. RHE as compared with a planar CdS/Au and pillar electrodes, respectively. A wide spectral range of enhancement was achieved, originating from photonic and plasmonic modes. Studies on the aspect ratio of P/TP and different thickness of CdS were carried out. The nanostructures are highly robust and can easily be utilized in other semiconductor thin film photovoltaic and photoelectrochemical cells.

O 77.19 Wed 18:15 Poster A

Metallic Phase-Change Materials for Nanoantenna Resonance Tuning — •Antonios Antonopoulos, Andreas F. Hessler, Martin Lewin, Tobias W. W. Mass, Matthias Wuttig, and Thomas Taubner — Institute of Physics (IA) RWTH Aachen

Nanostructured metasurfaces have the ability to manipulate light fields. Their properties depend on the size and position of nanostructures, which are generally fixed after fabrication.

Phase-change materials (PCMs) can be used to adjust the, otherwise fixed, properties of metasurfaces [1]. PCMs show a large contrast between their metastable crystalline and amorphous phases. So far, mainly PCMs that are dielectric in both phases in the infrared have been used [2].

Here, we apply a different kind of PCM to metasurfaces. In the infrared, In_3SbTe_2 (IST) is dielectric in the amorphous phase, but metallic in the crystalline phase. Simulations suggest that by switching IST deposited in the gap between neighboring nanostructures with a focused laser beam, we can conductively connect them. Moreover, we present results on metallic nanoantennas composed of crystalline IST which were directly written into a thin film of amorphous IST with a pulsed laser.

In general, metallic PCMs provide exciting new opportunities for the functionalization of metasurfaces.

[1] M.Wuttig et al., Nat. Photon. 11, 465 (2017)
[2] A.-K. U. Michel et al., Adv. Optical Mater. 5, 1700261 (2017)

O 77.20 Wed 18:15 Poster A

Investigation of antenna design for improving the number of switching cycles of phase-change material covered nanoantennas — •Achim Strauch, Andreas F. Hessler, Henrik Wördenweber, Matthias Wuttig, and Thomas Taubner — Institute of Physics (IA) RWTH Aachen

Phase-change materials (PCMs) have been shown to be a useful tool to provide metasurfaces with an active functionality. Since they generally have large optical contrasts between their metastable amorphous and crystalline phases, a change in the phase of a thin film of PCM ontop of a metasurface greatly influences its optical properties [1].

This phase-change can be controlled very locally around individual nanostructures with a focussed pulsed laser by either using long, low-energy or short, high-energy pulses for crystallization or amorphization, respectively. The transition between the two phases should be possible with a high number of switching cycles [2].

In our work, we investigate the influence of the design of nanostructures covered with the PCM $Ge_3Sb_2Te_6$ on the number of achievable switching cycles. Specifically, we compare rod with slit antennas and consider the influence of the thickness of a protecting capping layer.

A high number of switching cycles is an important prerequisite for nanophotonic applications of PCMs.

[1] M. Wuttig et al., Nat. Photon. 11, 465 (2017)
[2] M. Wuttig et al., Nat. Mater. 6, 824 (2007)

O 77.21 Wed 18:15 Poster A

Photon Correlation Measurements on Quantum Dots — •Lok-Yee Yan, Manuel Peter, and Stefan Linden — Physikalisches Institut, University of Bonn, Nußallee 12, D-53115 Bonn, Germany

Semiconductor quantum dots (QDs) can be used as single photon emitters in various applications. In our group we have developed a lithographic method that allows us to deposit a controllable number of colloidal semiconductor QDs on freely definable sites on the substrate. Lately, we improved this method to the reliable placement of single QDs which could be confirmed by electron micrographs. In order to demonstrate photon-antibunching of the fluorescence of a single QD, we are performing a Hanbury-Brown-Twiss experiment (HBT) which leads to the direct measurement of the second-order correlation function $g^{(2)}(\tau)$. In the HBT the fluorescence is divided by a 50:50 beam splitter and detected by two avalanche photodiodes. Both output signals of the photodiodes are fed into a Time-Correlated Single Photon Counting unit. The correlation function $g^{(2)}(\tau)$ can then be extracted by measuring the histogram of the time difference τ between the two signals. As a clear indicator for photon-antibunching, we expect a significant decrease of $g^{(2)}(0)$.

O 77.22 Wed 18:15 Poster A

Improved Dynamic Range Imaging in Time-Resolved 2PPE PEEM — •David Janoschka, Pascal Dreher, Michael Horn - von Hoegen, and Frank Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, Germany

The commonly used detector for low energy electron microscopy (LEEM) or photoemission electron microscopy (PEEM) is a combination of a multichannel plate (MCP) with a phosphor screen. An optical CCD or CMOS camera is then used to film the microscope image off the screen. In time-resolved imaging of nonlinear electron emission from strong plasmonic fields (Plasmoemission) such detection scheme reaches its limitations due to the high contrast and the dramatic intensity variations in the data on a sub-micrometer scale: simply due to the construction of a MCP/Screen combination, every bright small emission spot on the MCP is surrounded by a disc of slightly increased intensity ("halo"), which makes a quantitative analysis of the electron yield between two bright emission spots almost impossible. On the poster we report on a recent upgrade of the SPE-LEEM microscope at the University of Duisburg-Essen, during which the MCP/screen combination was replaced with a fiber-coupled CMOS sensor. We will show PEEM and LEEM images obtained with the new detector and we will compare the performance of the new detector with the previously used MCP setup. The new detector provides us with a much higher dynamic range, with less noise, and imaging without halos.

O 77.23 Wed 18:15 Poster A

Imaging with ultrathin nonlinear metalenses — •Christian Schlickriede[1], Philip Christian Georgi[1], Guixin Li[3], Shuang Zhang[2], and Thomas Zentgraf[1] — [1]Universität Paderborn, Paderborn, Germany — [2]School of Physics and Astronomy, University of Birmingham, United Kingdom — [3]Department of Materials Science and Engineering, Southern University of Science and Technology, China

In our approach we fabricate a new kind of plasmonic metalens, which is solely working in the nonlinear regime by instantaneous frequency conversion for the incident near-infrared light. Therefore, we use the concept of a nonlinear geometric phase emerging from the configuration of meta-atoms with specific rotational symmetry. The designed nonlinear metalenses are ultrathin devices with a thickness of only 30 nm. Depending on the incident circular polarization of light, the phase profile for the nonlinear harmonic generation process can be switched between convex and concave. In the experiments, we determine the formation of the real and virtual focal planes for illumination with Gaussian beams and we demonstrate nonlinear imaging abilities that giving rise to real and virtual images of real objects at visible wavelengths. Most importantly, we found that the nonlinear image evolution is not governed by the traditional lens equation but by a modified version of it.

O 77.24 Wed 18:15 Poster A

Ultrathin metasurfaces for nonlinear optical image encoding — •Felicitas Walter[1], Guixin Li[2], and Thomas Zentgraf[1] — [1]Department of Physics, University of Paderborn, D-33098, Germany — [2]Department of Materials Science and Engineering, Southern University of Science and Technology, Shenzhen, 518055, China

In this project we demonstrate that an ultrathin nonlinear photonic metasurface, consisting of meta-atoms with three-fold rotational symmetry, can be used to hide optical images under illumination with a fundamental wave. However, the hidden image can be read out from second harmonic generation (SHG) waves. This is achieved by controlling the destructive and constructive interferences of SHG waves from two neighboring meta-atoms. In addition, we apply this concept to obtain grey-scale SHG imaging. Nonlinear metasurfaces based on space variant optical interference open new avenues for multi-level image encryption, anti-counterfeiting and background free image reconstruction.

O 77.25 Wed 18:15 Poster A

On the resonances of an optical microcavity based on a hyperbolic metamaterial — •Thomas Kiel[1], Evgenij Travkin[1], Sergey Sadofev[1], Oliver Benson[1], Sascha Kalusniak[1], and Kurt Busch[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [2]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin

Metamaterials provide a rich variety of physical effects such as phase and group velocity control and negative refraction. Here, we present unusual resonance effects of a microcavity filled with a hyperbolic metamaterial (HMM). The HMM is based on pairs of stacked layers of epitaxially grown ZnO / ZnO:Ga.

We compare the experimental reflection spectra with numerical computations using the scattering-matrix algorithm. With the computation of the resonance states, a.k.a. quasi-normal modes, we gain a deeper understanding in the emergence of the cavities' resonances. We identify the different modes supported by computing their field distributions. Furthermore we can map out the modes' dispersion relation in good agreement with the experimental angular-resolved spectra. The tuning of the layer thicknesses and doping level of the HMM core allows us to tailor the modes of the system.

O 77.26 Wed 18:15 Poster A

Towards Superconducting Niobium Plasmonics for Light Detection — •Ahmed Farag, Shahin Bagheri, and Harald Giessen — 4th Physics Institute and Research Center SCOPE, University of Stuttgart, D-70550 Stuttgart, Germany

Nowadays with the fast developments in quantum computing and single photon emitters,avalanche photodiodes as photon detectors are replaced by the superconducting nanowire single-photon detectors. These detectors have a large active area, enabling high absorption efficiency but unfortunately, they slow down the detector response and increase the recovery time. To overcome this problem, plasmonic concepts can be combined with superconducting photon detectors to decrease the active area of the detector while maintaining the high absorption efficiency. Niobium is one of the most promising materials for such purpose since it has a reasonable transition temperature, low kinetic inductance, as well as promising plasmonic properties. Here, we study the optical properties of niobium and niobium nitride upon different sputtering conditions for plasmonics application. Two different nanofabrication techniques are used, namely, electron beam lithography for preparation of precise and complex designs and laser interference lithography for large-area nanostructures. Our results show tunability of the plasmon resonance and consequently the corresponding absorptions in the near infrared range. The absorption can be enhanced further to near unity using a perfect absorber design. The investigations into the plasmonic properties of superconducting niobium opens a gate for future single photon applications.

O 78: Poster: Surface Dynamics - Reactions, Elementary Processes and Phase Transitions

Time: Wednesday 18:15–20:30 Location: Poster A

O 78.1 Wed 18:15 Poster A

X-ray photoemission studies of the liquid metal catalyst Pd/Rh-Ga — •Haiko Wittkämper[1], Mathias Grabau[1], Jannis Erhard[3], Nicola Taccardi[2], Peter Wasserscheid[2], Christian Neiss[3], Andreas Görling[3], Hans-Peter Steinrück[1], and Christian Papp[1] — [1]Physikalische Chemie 2 — [2]Chemische Reaktionstechnik — [3]Theoretische Chemie, FAU Erlangen

Mixtures of Pd and Ga on porous silica were shown to be stable and selective alkane dehydrogenation catalysts. The beneficial effects of Ga addition to the active transition metal are due to the fact that the catalyst is in the liquid phase during reaction, which is indicated by SEM and XRD measurements, and termed supported catalytically active liquid metal solution (SCALMS).[1] We herein present XPS studies of Pd-Ga and Rh-Ga alloys as model systems for catalytically-active, supported liquid catalysts. In an effort to understand the underlying principles of the catalyst, the temperature-dependent Pd/Rh concentrations at the surface of the liquid phase were evaluated by quantitative XPS. The observed temperature-dependence is explained by the formation of transition metal-rich intermetallic phases, leading to the depletion of the liquid phase and the surface from the transition metal. For the Pd-Ga alloy, additionally, an inhomogeneous Pd distribution with depletion at the interface is suggested by ARXPS and DFT-based MD simulation. [2] Data on the Rh-Ga system will be presented and compared to the results obtained for the Pd-Ga alloy. [1] Taccardi, N., Grabau. M., et al. NatChem 9, 862-867 (2017). [2] Grabau. M., Erhard J., et al. ChemEurJ 23, 1-8 (2017).

O 78.2 Wed 18:15 Poster A

enhanced photocatalytic activities of net-like hematite nanoparticle modified with graphene oxide and mechanism insight — •huanming zhang[1], min zhou[1], yang xu[1], shipu xu[1], fanna meng[2], lihong qi[2], yujin chen[2], and yong lei[1] — [1]Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Key Laboratory of In-Fiber Integrated Optics, Ministry of Education, College of Science, Harbin Engineering University, 150001 Harbin, China

In photocatalytic water oxidation, hematite possesses many attractive features, for instance favorable optical band gap (approximately 2.1 eV), chemical stability, natural abundance, nontoxicity and low cost. However, its sluggish surface reaction kinetics, short carrier lifetime and considerably shorter diffusion length of holes compared with the absorption depth hold back its practical application. Thus, A co-catalyst may be an effective way to remedy these drawbacks. Herein, a facile strategy was developed to fabricate net-like hematite nanoparticle (NHN) modified with graphene oxide (GO), in which the degree of oxidization of GO could be controlled by simply changing annealing time, and GO replaces part of hematite as the reaction interface to speed up the oxygen evolution rate. NHG with GO of appropriate oxidization degree and content exhibited much higher photocatalytic activities than hematite nanorods and commercial hematite. The strategy presented here could be expanded as a general method to synthesize other types of photocatalysts modified with GO for applications in photocatalysis.

O 78.3 Wed 18:15 Poster A

Utilization of coke oven gas for the catalytic production of methane and methanol — •Fabian Rachow, Klaus Müller, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus - Senftenberg, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

Coke oven gas (COG) is a byproduct in the production of carbon rich coke from coal for the steel industry. Apart from a high amount of hydrogen (~60vol%) and methane (~25vol%), COG contains CO (5-8vol%) and CO_2 (1-3vol%), thus making it an attractive feedstock for the production of synthetic energy carriers like methane and methanol via catalytic conversion. The conventional route requires steam reforming of the methane to syngas for further reaction. We however investigate a different approach to directly convert the CO and CO_2 from COG to methane and/or methanol. The process is evaluated by the conversion of CO and CO_2, yield of CH_4 and CH_3OH and selectivity towards higher hydrocarbons for varying temperature and pressure. A surplus of hydrogen in the COG might be compensated by additional CO_2 from air, flue gas or coal gasification to achieve a higher yield.

O 78.4 Wed 18:15 Poster A

Segregation Study of Size-Selected Bimetallic Nickel-Cobalt Nanoparticles for Partial Oxidation of Methane — •Peter Franz Zajac[1], Ioannis Zegkinoglou[1], Lukas Pielsticker[1], and Beatriz Roldan Cuenya[1,2] — [1]Department of Physics, Ruhr University Bochum, 44780 Bochum, Germany — [2]Department of Interface Science, Fritz-Haber Institute of the Max Planck Society, Berlin 14195, Germany

Alloying and segregation phenomena in bimetallic nanoparticle catalysts crucially affect their elemental surface composition and are often responsible for synergistic effects which enhance their catalytic performance in comparison to their monometallic counterparts. We used *in situ* X-ray photoelectron spectroscopy, both in ultra-high vacuum and under near-ambient pressure conditions (NAP-XPS), in combination with atomic force microscopy (AFM), to investigate the morphological stability, chemical state and surface composition of size-selected bimetallic nickel-cobalt nanoparticles supported on silicon dioxide substrates as a function of temperature and gas environment for the catalytic partial oxidation of methane (CPOM). The studies demonstrated the remarkable stability of surface cobalt oxide species under reducing conditions and indicate that pretreatment of the nanocatalysts by plasma etching or annealing can help tune their catalytic properties.

O 78.5 Wed 18:15 Poster A

Modeling Nonadiabatic Effects in Gas-Surface Dynamics by Means of Electronic Friction — •Simon P. Rittmeyer and Karsten Reuter — Technische Universität München

Energy transfer at and across the interface fundamentally governs the dynamics of surface chemical reactions, e.g., in heterogeneous catalysis. On frequently employed metal catalysts, likely dissipation channels are the adsorbate interaction with substrate phonons and the nonadiabatic excitation of electron-hole (*eh*)-pairs in the surface. Despite considerable effort spent in the past decades, however, a general assessment of the relative importance of these competing energy dissipation channels has still not been achieved. In parts, this is attributable to the uncertainty that comes with effective models for the nonadiabatic energy dissipation—such as the electronic friction approach—inevitable for large scale simulations.

In order to improve upon this situation, we demonstrate the validation of the popular local density friction approximation (LDFA) for electronic friction by comparing to experimentally measured vibrational lifetimes [1], scrutinize underlying assumptions using explicitly evaluated *eh*-pair excitation spectra [2], and ultimately invoke this effective model to disentangle the role of the competing energy dissipation mechanisms in the context of thermal adatom diffusion [3].
[1] S.P. Rittmeyer *et al.*, Phys. Rev. Lett. **115**, 046102 (2015).
[2] S.P. Rittmeyer *et al.*, Phys. Rev. Lett. **119**, 176808 (2017).
[3] S.P. Rittmeyer *et al.*, Phys. Rev. Lett. **117**, 196001 (2016).

O 78.6 Wed 18:15 Poster A

Dynamics and reactivity of long-lived excess electrons in DMSO films on Cu(111) — •Angelika Demling, Sarah B. King, Katharina Broch, and Julia Stähler — Department of Physical Chemistry, Fritz Haber Institute of the MPG, Faradayweg 4-6, 14195 Berlin, Germany

DMSO is a widely used non-aqueous solvent with the potential to be used in lithium-oxygen batteries due to its ability to catalyze the superoxide formation and to stabilize the products. In this work we investigate the electron dynamics in DMSO films on Cu(111) using time-resolved two-photon photoemission. We show that films of a thickness > 2 monolayers exhibit two surface-bound electronic states at 2.41 ± 0.05 eV and 2.30 ± 0.05 eV above the Fermi level with lifetimes on the order of several seconds. Both are formed from the same precursor state, a small polaron in the second monolayer. Due to their long lifetime and binding location on the DMSO surface, we assign these states to electrons residing in deep traps at the DMSO/vacuum interface. Moreover, the photoemission signal from the trapped electrons decreases and the work function increases over time under illumination. Both effects are disscussed as possible results of light-induced reorganization of molecules at the surface. Further experiments in an oxygen atmosphere suggest the surface-bound electrons react with oxygen, making these findings of high relevance for the understanding of the formation of superoxide in lithium-oxygen batteries.

O 78.7 Wed 18:15 Poster A

New molecular beam set-up to study dynamics at ionic liquids surfaces — •Radha Gobinda Bhuin, Hans-Peter Steinrück, and Florian Maier — Lehrstuhl für Physikalische Chemie II, FAU, Erlangen, Germany

More than a decade surfaces and interfaces of ionic liquids (ILs) have been studied extensively. These studies mostly concern 'static' properties of ILs such as interface composition, molecular orientation and surface termination, enrichment and layering effects, surface tension, and adsorption of small molecules.1,2,3 However, the dynamics of the transfer of the gases through the interface and its dependence on the interface properties have not been studied so far, despite their importance in catalysis and separation technologies.4 Therefore, to investigate the dynamical interaction processes at the ionic liquid surfaces we have designed and built a new molecular beam setup which combines a supersonic molecular beam with a rotatable mass spectrometer and an X-ray photoelectron spectrometer for in situ XPS-investigations. Using this set-up we will address in particular the question how gases pass through the gas/liquid interface depending on the gas / IL physicochemical properties. RGB and HPS thank the ERC for financial support through an Advanced Investigator Grant to HPS. References [1] H.-P. Steinrück, Phys. Chem. Chem. Phys. 14, 5010 (2012). [2] H.-P. Steinrück, Surf. Sci. 604, 481 (2010). [3] K. R. J. Lovelock et al., Chem. Rev. 110, 5158 (2010). [4] N. V. Plechkovaa and K. R. Seddon, Chem. Soc. Rev. 37, 123 (2008).

O 78.8 Wed 18:15 Poster A

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

Artificial molecular motors can translate an external stimulus into controlled motion. They have seen great developments in the last decades [1]. While many studies exist in solution, only very little is known how such functional molecules behave on a surface, although such a setup holds the advantage of a fixed point of reference. This is of importance for a key property of molecular machines, the directionality of their motion in a static environment.

In this study, artificial motor molecules have been investigated, all based on a combination of double bond isomerization and helix inversion, which are the key processes responsible for rotation of the so-called Feringa motor. This type of motor has already been used to successfully drive lateral translation of molecules at surfaces [2, 3]. Experiments were done by low temperature scanning tunneling microscopy (STM) to enable imaging of one and the same molecule before applying an external stimulus. The focus of our study is on the adsorption of such molecules at metallic surfaces and what type of motion can be induced by either STM manipulation or illumination by light.

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

O 78.9 Wed 18:15 Poster A

Model catalytic studies of liquid organic hydrogen carriers: Pyridine / piperidine on Ni(111) — •Marie Freiberger, Johann Steinhauer, Philipp Bachmann, Florian Späth, Udo Bauer, Fabian Düll, Hans-Peter Steinrück, and Christian Papp — Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

A strong effort for the implementation of renewable energy sources was made by constructing large-scale wind farms and solar plants, which replace power plants with non-renewable fuels. The availability of these energy sources is unsteady and unpredictable due to environmental influences. Therefore, energy storage becomes more important in the near future. One concept is the use of liquid organic hydrogen carriers (LOHC), which enable hydrogen storage under ambient conditions. In an LOHC system, when excess energy is available, organic molecules are catalytically loaded with hydrogen to form an energy- and hydrogen-rich compound. Afterwards, when energy is needed, hydrogen is catalytically unloaded and the hydrogen lean form is restored. Herein, we present detailed studies on the LOHC system pyridine and its hydrogenated form piperidine. This LOHC system is investigated in a model catalytic approach on a Ni(111) surface under ultra-high vacuum conditions. Using synchrotron radiation-based high-resolution X-ray photoelectron spectroscopy we are able to observe the adsorption, desorption and reaction behaviour of the LOHC system. Furthermore, insights on the structure-reactivity relationship in dehydrogenation catalysis of heterocyclic compounds are provided.

O 78.10 Wed 18:15 Poster A

Motorized molecules studied by scanning tunneling microscopy — •Peter Jacobson[1], James M Tour[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, 8010 Graz, Austria — [2]Department of Chemistry, Rice University, Houston, Texas 77005, USA

Motorized molecules are envisioned as cargo carriers at the nanoscale. Critical to their success is the controlled activation of motion using external stimuli. In Feringa type motors, UV light triggers a sequence of isomerization and helical inversion steps leading to the unidirectional rotation of the motor. When incorporated into larger molecules, these motors are a potential source of unidirectional translation at surfaces. Scanning probe microscopy is an ideal tool to investigate the single molecule dynamics of these molecular machines, but commonly used metal substrates have drawbacks, such as the quenching of excited states by conduction electrons. An alternate approach is to deposit them on semiconducting substrates, thereby reducing the adsorption strength of the molecule on the surface and removing a potential path for quenching. Here, I will present initial results on motorized molecules containing a Feringa motor on semiconducting surfaces.

O 78.11 Wed 18:15 Poster A

On the kinetics of the self-metalation reaction of 2H-tetraphenylporphyrin derivatives on Cu(111) with different peripheral CN functionalization — •Manuel Meusel, Michael Lepper, Julia Köbl, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany.

In this contribution, we present a detailed scanning tunneling microscopy (STM) study concerning the kinetics of the self-metalation reaction of 2H-tetraphenylporpporphyrins (2HTPP) on Cu(111) with and without peripheral cyano functionalization. The corresponding self-metalation reaction, in which the free base porphyrins metalate with Cu atoms from the substrate, has been studied intensively for 2HTPP on Cu(111) in the past [1-3]. Surprisingly, we observed a strong decrease of the self-metalation rate directly correlating to the degree of functionalization with peripheral cyano groups, opposed to the expected trend for a metalation in solution. Statistical analysis of isothermal STM time series allows for the estimation of corresponding changes in the activation energy of the self-metalation for the different porphyrin species. The origin of this phenomenon will be discussed in respect to different binding motifs and the intramolecular conformation of the porphyrins. This work was funded through DFG FOR 1878 (funCOS) under grant MA 4246/2 -1. [1] K. Diller et al., J. Chem. Phys., 136 (2012) 014705 [2]S. Dietze et al., Ang. Chem. Int. Ed. 51 (2012) 10898 [3] H. Marbach, Acc. Chem. Res., 48 (2015) 2649

O 78.12 Wed 18:15 Poster A

Reactivity of benzene on a sulfur-passivated Pt(111) surface — Johann Steinhauer, Philipp Bachmann, Udo Bauer, Florian Späth, Fabian Düll, Hans-Peter Steinrück, and •Christian Papp — Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Egerlandstr.3, 91058 Erlangen, Germany

Poisoning of catalysts with sulfur is a major issue in large scale applications. One very efficient poison for catalysts is sulfur, which leads to the blocking of reactive sites and a strong reduction of the total adsorption capacity. Interestingly sulfur is also used as a promoter in the dehydrogenation reaction of hydrocarbons. To understand the particular influence of sulfur in this reaction, we studied the effect of sulfur contamination on the reaction behavior of benzene on a Pt(111) single crystal with Temperature Programmed Desorption (TPD) and synchrotron based high-resolution XPS. In these studies, the sulfur coverages were varied up to 0.3 ML, obtained by adsorbing H_2S and subsequent annealing to 500 K. We followed the reaction of benzene on Pt(111) as a function of sulfur coverage. For sulfur-poisoned surfaces we find the desorption of benzene occurs at slightly lower temperatures of about 400 K. On the sulfur free Pt(111) surface also the reaction and decomposition is found at higher temperatures of 435 and 640 K, respectively. This effect of sulfur on the reaction was also found in TPD measurements. Sulfur leads to a shift of the desorption peaks to lower temperatures with increasing sulfur coverages. Thereby indicating a decreased binding energy between catalyst and substrate or a deactivation of active sites on the catalyst through sulfur poisoning.

O 78.13 Wed 18:15 Poster A

Model Catalytic Studies of Liquid Organic Hydrogen Carriers: Dehydrogenation of Indole, Indoline and Octahydroindole on Pt(111) — Philipp Bachmann[1], Johann Steinhauer[1], Florian Späth[1], Fabian Düll[1], Udo Bauer[1], Marlene Scheuermeyer[2], Peter Wasserscheid[2], Hans-Peter Steinrück[1], and •Christian Papp[1] — [1]Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen, Germany — [2]Lehrstuhl für Chemische Reaktionstechnik, FAU Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen, Germany

Indole derivatives are considered promising Liquid Organic Hydrogen Carriers (LOHC) for renewable energy storage. Using X-ray photoelectron spectroscopy (XPS) and Temperature Programmed Desorption (TPD), we investigated low temperature adsorption, and dehydrogenation during heating of the hydrogen-lean indole, as well as the hydrogen-rich indoline and octahydroindole on Pt(111). For all three molecules, we find deprotonation of the NH bond above 270 K. For the hydrogen-rich carrier molecules indoline and octahydroindole we find that this deprotonation is accompanied by dehydrogenation via an indole intermediate, resulting in an indolide species above 300 K. For octahydroindole, we also find a side reaction yielding small amounts of a π-allyl species between 170 and 450 K. Above 450 K, decomposition of the remaining indolide species takes place.[1]

[1] M. Schwarz, P. Bachmann et al., Chem. Eur. J., 2017, 23, 14806-14818.

O 78.14 Wed 18:15 Poster A

Observing oxide surface reactivity at high temperatures: FastSTM on Fe_3O_4(001) — •Alexander Bourgund, Barbara A. J. Lechner, Ueli Heiz, and Friedrich Esch — Department of Chemistry & Catalysis Research Center, Technical University of Munich, Lichtenbergstr. 4, D-85748 Garching

Magnetite as a highly abundant oxide material shows a rich surface chemistry and is a well-known support for nanoparticles in catalysis [1]. While its surface dynamics have been studied extensively with conventional Scanning Tunneling Microscopy (STM) and other techniques [1-3], little is known about these surface processes at the atomic scale when studied at elevated temperatures, with the required high temporal resolution. We present results on magnetite Fe_3O_4(001) surface dynamics taken with a specially developed FastSTM add-on module [4] that boosts the temporal resolution of our commercial STM up to 12 frames/s. In particular, we resolve subsurface diffusion of iron atoms and their exchange with the bulk at temperatures up to 800 K and provide additional insight into the high-temperature transition [3]. Furthermore, we observe surface etching under reducing or wet conditions, as well as growth in an oxygen atmosphere. The reactivity of the surface can be enhanced by deposition of Pt_{10} clusters that lower the reaction onset temperature.

References: [1] G. S. Parkinson, *Surf. Sci. Rep.* 2016, *71*, 272. [2] R. Bliem *et al.*, *Angew. Chem. Int. Ed.* 2015, *54*, 13999. [3] N. C. Bartelt *et al.*, *Phys. Rev. B* 2013, *88*. [4] F. Esch *et al.*, *Rev. Sci. Instrum.* 2011, *82*, 53702 and NFFA project JRA1.

O 78.15 Wed 18:15 Poster A

Analysis and interpretation of TPD measurements of organic molecules — •Karolina Stoiber, Peter Deimel, Julian Lloyd, Francesco Alegretti, Joachim Reichert, Hartmut Schlichting, and Johannes V. Barth — Physics Department, Technical University of Munich, James-Franck-Straße 1, 85748 Garching, Germany

In surface science, thermal programmed desorption (TPD) is one of the most traditional measuring techniques for the investigation of adsorbed species. Typically, a well-defined substrate covered with the molecules under investigation is heated up with a constant heating rate. Depending on kinetic parameters and the arrangement on the surface, desorption occurs at distinct temperatures with characteristic rates, until the substrate is depleted. Moreover, the interpretation of TPD spectra requires additional information gathered from methods like scanning tunnelling microscopy (STM). We realized a setup consisting of a TPD chamber flanged to a STM unit and a controlled ion beam deposition (CIBD) system to investigate large functional molecules and their assemblies on clean substrates. The TPD chamber provides a STM-compatible sample holder which can be cooled down to liquid nitrogen temperatures and heated up to some 1500 K for measuring. A quadrupole mass spectrometer, with a Feulner cup enhancing the desorbing flux of molecules, monitors the desorption rate. Together with the recorded temperature, binding energies and preexponentials of bisphenol A and diethylstilbestrol on Cu(111) are extracted and the TPD spectra are simulated with analytical and Monte Carlo methods.

O 79: Poster: Ultrafast Electron and Spin Dynamics at Interfaces

Time: Wednesday 18:15–20:30 Location: Poster A

O 79.1 Wed 18:15 Poster A

Charge transfer dynamics in monomolecular films: azulene and polyacene backbones, pyridine as a resonantly addressable group — Tobias Wächter[1], Andreas Terfort[2], Mikhail V. Barybin[3], and •Michael Zharnikov[1] — [1]Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [2]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, 60438 Frankfurt, Germany — [3]Department of Chemistry, University of Kansas, Lawrence, Kansas 66045-7582, USA

We review recent progress in the application of core hole clock approach in the framework of resonant Auger electron spectroscopy to the monomolecular assembles to study electron transfer (ET) dynamics in these systems serving as prototypes of molecular electronics devices. The ET pathway to the substrate was unambiguously defined by resonant excitation of the specific tail group (nitrile) attached to the molecular backbone. Characteristic ET times within the femtosecond domain were determined, along with the attenuation factors for the ET dynamics, analogous to the case of the static transport. Three different systems were studied. The first system was 2-mercapto-6-cyanoazulene monolayer which is of importance in view of a possible correlation between the ET dynamics and molecular dipole moment. The second systems were monolayers with the acene backbone which are of importance in view of the existing controversy regarding the attenuation factor for this specific type of molecular films. The third system was a series of pyridine-substituted monolayers where, instead of nitrile, the pyridine moiety was used as the starting point for ET to the substrate.

O 79.2 Wed 18:15 Poster A

Momentum dependent hot electron lifetimes in metals — •Tobias Eul[1], Florian Haag[1,3], Philip Thielen[1,3], Martin Feidt[1], Mirko Cinchetti[2], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,3] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Germany — [2]Experimentelle Physik VI, Technische Universität Dortmund, Germany — [3]Graduate School MAINZ, Germany

Understanding the correlation between the electronic band structure and the corresponding hot carrier dynamics is of utmost importance to improve the performance of next-generation electronic and spintronic devices. In this context, we will combine momentum microscopy with two-photon photoemission to directly image the momentum dependent electron dynamics of 2D materials and metal-organic systems.

In a first step, we have chosen to study the electron dynamics of noble metals with the combination of our photoemission electron microscope with a time-of-flight detector. The experimental data obtained by time-resolved two-photon momentum microscope can be used to directly translate the transient photoemission yield into intermediate state lifetimes.

For Ag single crystals, we observe a clear momentum dependence of the electron lifetimes for all intermediate state energies. These findings are discussed in the light of static one and two photon momentum microscopy experiments which allow us to characterize the electronic states involved in the optical excitation process.

O 79.3 Wed 18:15 Poster A

Time-domain identification of electronic correlations in $1T$-TaS$_2$ — Manuel Ligges[1], Isabella Avigo[1], Denis Golež[2], Hugo Strand[2], •Yasin Beyazit[1], Kerstin Hanff[3], Florian Diekmann[3], Ljupka Stojchevska[1], Matthias Kalläne[3], Ping Zhou[1], Kai Rossnagel[3], Martin Eckstein[4], Phillip Werner[2], and Uwe Bovensiepen[1] — [1]Faculty of Physics, Universität Duisburg-Essen — [2]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [3]Institute of Experimental and Applied Physics, Universität Kiel, 24098 Kiel — [4]Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL, 22761 Hamburg

We used time-resolved photoemission spectroscopy to isolate and access fundamental Mott-physics in the (quasi) 2D transition-metal dichalcogenide $1T$-TaS$_2$. Doublon-holon recombination is found to occur on time scales as short as only a few electronic hopping cycles $\hbar/J$. Despite strong electron-phonon coupling, the dynamics can be reproduced within a single-band Hubbard model in the absence of additional bosonic coupling channels. We furthermore find that hole-doping governs the relaxation dynamics on ultrashort time scales.

O 79.4 Wed 18:15 Poster A

Time-resolved momentum microscopy using a high-repetition rate HHG lightsource — •David Schmitt, Marius Keunecke, Christina Nolte, Daniel Steil, Sabine Steil, and Stefan Mathias — I. Physikalisches Institut Göttingen, 37077 Göttingen, Friedrich-Hund-Platz 1

Recent developments in laser technology and electron spectrometers allow for the build-up of a new generation of time-resolved photoelectron emission experiments. With regard to lightsource development, coherent extreme-ultraviolet femtosecond pulses can today routinely be produced via high-harmonic generation at repetition rates up to 1 MHz, which is essential in time-resolved photoemission spectroscopy/microscopy to avoid space charge effects. In addition, new and highly-efficient electron spectrometers are available that map the full parallel momentum space of the electronic structure (ARPES), or can be used as photoemission electron microscopes (PEEM) with several tenths of nanometers spatial resolution. On our poster, we will present first measurements with such a combined time-resolved photoemission setup. We will discuss detection efficiency, space charge effects and energy-, time-, momentum- and spatial resolution that can be achieved.

O 79.5 Wed 18:15 Poster A

Time-resolved photoemission tomography of organic thin films — •Sebastian Hedwig[1], Sebastian Emmerich[1,2], Johannes Seidel[1], Dominik Jungkenn[1], Florian Haag[1], Christina Schott[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany

Photoemission tomography is a powerful method to correlate the momentum resolved photoemission yield of organic thin films to the shape of the molecular orbitals in real space [1]. Using static light sources, this technique has been successfully used to identify the emitting molecular orbitals of metal-organic interfaces or to determine the density of states of different molecules in heteromolecular structures [2]. Here, we extend this approach to the ultrafast timescale. By combining momentum microscopy with fs-XUV light sources, we are able to directly image the time-resolved evolution of occupied molecular orbitals and to access the momentum space pattern of unoccupied molecular orbitals. Here, we present our first results of the optically induced transient behavior of the momentum space signature of molecular orbitals of a C_{60} thin film. These results will be analyzed in the photoemission tomography approach to gain insight into transient changes of the molecular orbital during and after the optical excitation.

[1] Science 326 702 (2009), [2] Nat. Commun. 5, 3685 (2014)

O 79.6 Wed 18:15 Poster A

High-repetition rate extreme ultraviolet HHG light source for femtosecond surface science experiments — •Christina Nolte[1], Amelie Schulte[1], Marco Merboldt[1], Germaine Arend[1], Steffen Hädrich[2], Tino Eidam[2], Jens Limpert[2], Sabine Steil[1], Daniel Steil[1], and Stefan Mathias[1] — [1]1st Physical Institute, University of Göttingen — [2]Active Fiber Systems GmbH, Jena

Table-top coherent ultrashort extreme ultraviolet light sources from high-harmonic generation have been shown to enable a wealth of novel experiments in the field of ultrafast surface science [1,2]. However, the full potential of this approach has not yet been achieved because, to date, high harmonics generated by low-repetition rate Ti:sapphire lasers required a trade-off between photon flux, repetition rate, energy and time resolution [3]. Here, we present a HHG light source driven by a nonlinearly compressed 0.5 MHz fiber laser enabling $> 10^{10}$ photons/s in single harmonics between 22-73 eV. In addition, our setup enables the direct generation of harmonics with bandwidths of the order of about 50 meV, so that the light source is ideally suited for next generation femtosecond spin- and angle-resolved photoemission experiments.

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

[2] Mathias et al., JESRP 189, 164 (2013)
[3] Eich et al., JESRP 195, 231 (2014)

O 79.7 Wed 18:15 Poster A

Development of a tabletop femtosecond broadband soft X-ray source — •Oscar Naranjo-Montoya, Manuel Bridger, Alexander Tarasevitch, and Uwe Bovensiepen — Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, Germany

Pump-probe experiments with optical excitation and absorption spectroscopy in the soft X-ray range on a femtosecond timescale are useful to analyze electronic and magnetic properties of complex material systems and their temporal evolution. These experiments have become available at Free Electron Laser and Synchrotron sources. However, due to the limited accessibility of these large scale facilities, systematic studies remain arduous to perform. Therefore, it will be useful to develop compact laboratory based sources. A promising approach is to use high harmonic generation in noble gases driven by mid-infrared femtosecond pulses. It has already been shown that with such radiation it is possible to generate photon energies that reach the keV regime [1]. We present the development of a high power two stage Optical Parametric Chirped-Pulse Amplifier as a pump for a tabletop soft X-ray source dedicated to absorption spectroscopy. 1 ps pump pulses at 515 nm amplify seed pulses at 800 nm by a factor of 20000. Their wavelength is converted to 1500 nm with a bandwidth of 40 nm and energy of 10 mJ. The 1500 nm pulses are the seed to produce λ=3200 nm with 100 fs duration. The achieved spatial, spectral and temporal pulse characteristics and an estimate of the soft X-ray flux will be presented. This work is funded by the DFG through SFB 1242, TP A05. [1] T. Popmintchev et al., Science **336**, 1287-1291 (2012).

O 79.8 Wed 18:15 Poster A

A novel setup for XUV-based time-resolved ARPES at 500 kHz repetition rate — M. Puppin, C. Nicholson, P. Xian, W. Windsor, Y. Deng, J. Feldl, C. Monney, M. Wolf, •L. Rettig, and R. Ernstorfer — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

We present a novel setup for time- and angle-resolved photoemission spectroscopy (trARPES) based on ultrashort extreme ultraviolet (XUV) laser source with 0.5 MHz repetition rate. The source is driven by an optical parametric chirped pulse amplifier (OPCPA) based on a hybrid fiber-slab amplifier system. The near-infrared OPCPA output is frequency-upconverted sequentially: frequency-doubling to 3.1 eV photon energy is followed by 7th harmonic generation (21.7 eV) in a dense noble gas jet. After spectral filtering, an XUV pulse with 20 fs pulse duration, a bandwidth of $\sim$ 100 meV and a photon flux exceeding 10^{11} photons/s is available for trARPES.

We demonstrate the capabilities of the setup by mapping the excited state structure of bulk WSe$_2$ 100 fs after optical excitation with 3.1 eV photons throughout the Brillouin zone and compare the results to DFT band structure calculations. Furthermore, in TbTe$_3$ we investigate the closing of the charge density wave energy gap and unfolding of the band structure in both occupied an unoccupied states after excitation with 1.55 eV photons. Our experimental setup allows the observation of occupied and transiently populated unoccupied states and their dynamics in the whole Brillouin zone, and the determination of direct and indirect band gaps within a single experiment.

O 79.9 Wed 18:15 Poster A

Time-resolved time-of-flight momentum microscopy at femtosecond lab sources — •Eva Sophia Walther[1], Tobias Eul[1], Florian Haag[1,2], Katerina Medjanik[3], Gerd Schönhense[3], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Germany — [3]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

Time and angle-resolved photoemission spectroscopy (trARPES) is one of the most important tools to investigate ultrafast carrier dynamics in solids. The largest challenge in trARPES is the small angular acceptance of conventional hemispherical electron analysers which only allows one to image a small part of the Brillouin zone. This limitation can be overcome by momentum microscopy, as recently shown at the free-electron laser FLASH [1]. This technique uses a set of parallel-imaging optics designed for best resolution in k-space. In combination with ToF data recording it allows to collect the photoelectron distribution in the full hemisphere above the sample surface and the complete d-band complex in a single acquisition. Here, we present the first results obtained with our newly commissioned ToF-momentum microscope which was combined with fs-laser light sources. The status of the development will be demonstrated by first 2PPE momentum microscopy data obtained for noble metal surfaces and ferromagnetic thin films. Finally, we will discuss possibilities for ToF-momentum microscopy with fs-XUV light sources. [1] H.-J. Elmers et al., this conference

O 79.10 Wed 18:15 Poster A

Photoexcitation of doublons in $1T$-TaS$_2$ — •Y. Beyazit[1], J. Beckord[1], I. Avigo[1], M. Ligges[1], M. Kalläne[2], P. Zhou[1], K. Rossnagel[2], and U. Bovensiepen[1] — [1]Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany — [2]Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany

Layered two-dimensional materials such as transition metal dichalcogenides exhibit rich phase diagrams. $1T$-TaS$_2$ is metallic at high temperatures, while below 180 K it becomes an insulator and the topmost electronic band splits due to a commensurate periodic lattice distortion into an occupied lower (LHB) and an unoccupied upper Hubbard band (UHB), separated by a 350 meV energy gap. The UHB can be populated by generating doublons with femtosecond laser pulses whose photon energy (1.55 eV) largely exceeds the electronic band gap, raising questions on the underlying excitation mechanism [2-4]. Using femtosecond time- and angle-resolved photoemission with different pump photon energies we find that upon excitation with 1.55 eV photons the UHB is observed, pumping with 0.92 eV and 1.04 eV results in a suppression of the UHB signature. We conclude that for the generation of a doublon population in the UHB a resonant dipole transition from an initial state is required, which is not the case for pumping with the lower photon energy. This confirms a dipole-like excitation scheme proposed recently [4].

[1] Sipos et al., Nature Mater. **7**, 960 (2008), [2] M. Ligges et al., arXiv:1702.05300 (2017), [3] N. ten Brinke et al., PRB **95**, 195123 (2017), [4] A. Mann et al., PRB **94**,115122 (2016)

O 80: Poster: Scanning Probe Techniques - Method Development

Time: Wednesday 18:15–20:30 Location: Poster A

O 80.1 Wed 18:15 Poster A

Thermally induced sharpening of tungsten STM-tips — •Timm-Florian Pabst, Hendrik Bettermann, and Mathias Getzlaff — Institute of Applied Physics, Heinrich-Heine-Universität Düsseldorf

Scanning Tunneling Microscopy (STM) allows to investigate structures with a lateral resolution down to the atomic scale. Special attention should be paid to the differing quality or sharpness of the used tip.

The goal of this work is to improve the quality of etched tungsten-STM-tips by using electron-bombardment heating. The resulting sharpness is investigated by testing the tips on tungsten oxide $(O-((1\times1)\times12))$ structure, and FeCo- and Co-nanoparticles deposited on a W(110) surface. The nanoparticles have a size of 3 nm to 9 nm and are produced in situ with a Magnetron Aggregation Source (Haberland type) and an Arc Cluster Ion Source. All measurements are carried out under ultra-high vacuum conditions at room temperature.

O 80.2 Wed 18:15 Poster A

Development of a fibre-based interferometer for an aperturless Scanning Near-field Optical Microscope — •Patrick Pietsch, Jonas Albert, and Markus Lippitz — University of Bayreuth, Bayreuth, Germany.

Aperturless scanning near-field optical microscopy (aSNOM) is a technique to measure the electric near-fields of nanoobjects, such as plasmonic structures, with deep subwavelength resolution. For this purpose an interferometer is required to obtain information on amplitude and phase of the near-field.

We will show how stability and signal-to-noise ratio of these experiments could be improved by using a fibre-based Mach-Zehnder interferometer, instead of a setup based on free space optics. Furthermore we will show, how it helps to increase the ease of use of this experiments.

O 80.3 Wed 18:15 Poster A

Design of a cryogenic dip-stick tuning fork-based AFM/STM system — •christian salazar, heiko hädrich, danny baumann, thomas mühl, bernd büchner, and christian hess — Leibniz Institute for Solid State and Materials Research, Dresden, Germany

We present the design of a tuning fork-based AFM/STM system, which consists in a dip-stick device able to operate inside a helium dewar or a magnet bath cryostat. The design allows to use in the AFM mode a frequency modulation feedback loop instead of the typical optical feedback loop. Additionally, this design provides the opportunity to connect a conducting tip to one of the tuning fork electrodes in order to run the STM mode. Measurements can be carried out in the temperature range from approximately 4K to room temperature and under cryogenic vacuum conditions. The system includes a cleaving mechanism for cleaving single crystals and a capacitive automated coarse approach mechanism for bringing the tip close to the sample surface without tip or surface damage.

O 80.4 Wed 18:15 Poster A

Etching tungsten nanotips using nitrogen gas in a field ion microscope — •Alexander Ihle, Sören Zint, Daniel Ebeling, and André Schirmeisen — Institute of Applied Physics, Justus Liebig University Giessen, Germany

Ultra-sharp tungsten nanotips are used in various applications. For low temperature atomic force microscopes, e.g., where quartz tuning forks are used as sensors nanotips are often fabricated from thin tungsten wire. To achieve ultimate lateral resolution or for functionalizing the tips with single CO molecules extremely sharp tips with radii in the nm or even in the sub-nm regime are needed. In 2006 Rezeq et al. [1] introduced a new method for tip fabrication, where electrochemically etched tungsten tips are further sharpened in a subsequent step by field-assisted etching with nitrogen gas. Therewith, tip radii below 1 nm can be reproducibly fabricated. Here, we are analyzing the effect of the nitrogen pressure on the tip etching process. To precisely determine the tip radius we use the so-called *feature size mapping* method [2]. Our measurements reveal that the tip radius decreases linearly in time for various nitrogen gas pressures in a range between 5.6 x 10-8 mbar and 5 x 10-6 mbar. Therefore, the etching rate at a specific pressure is constant. Furthermore, it is demonstrated that the etching rates increase linearly with higher nitrogen pressures, which allows us to precisely estimate the process time.

[1] Rezeq et al. *The Journal of Chemical Physics* **124**, 204716 (2006)

[2] Zint et al. *Phys. Rev. B* **90**, 241413 (2014)

O 80.5 Wed 18:15 Poster A

Design and performance of a UHV spin-polarized STM operating at 30 mK in vector magnetic fields — •Henning von Allwörden[1], Elze J. Knol[1], Andreas Eich[1], Jan Hermenau[2], Andreas Sonntag[2], Jan W. Gerritsen[1], Daniel Wegner[1], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [2]Fachbereich Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

Scanning tunneling microscopy (STM) has developed into a leading technique to explore atomic-scale magnetism. However, to enhance the energy resolution in order to probe spin-dependent phenomena, our instrument design is based on a wet dilution refrigerator. Its base temperature is around 30 mK and it is capable of vector magnetic fields in two dimensions. The connection to an ultra-high vacuum (UHV) system allows in-situ sample preparation and transfer. The setup is situated in an ultra-quiet and ultra-low noise laboratory (SPiN laboratory at the IMM in Nijmegen), and also special care was taken to do signal filtering in-situ. We demonstrate the instrumentational performance by showing the noise characteristics at the tunnel junction, atomic resolution of a surface and measured quasi-particle interference (QPI), showing the ability to perform QPI mapping. Furthermore, we illustrate spectra of low temperature BCS superconductors and discuss the electron temperature.

O 80.6 Wed 18:15 Poster A

Four-point probe measurements using current probes with voltage feedback to measure electric potentials — •David Cuma[1,2], Felix Lüpke[1,2], Stefan Korte[1,2], Vasily Cherepanov[1,2], and Bert Voigtländer[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-FIT, 52425 Jülich, Germany

Four-point probe sensing is a widespread measurement technique to determine electrical impedances. The underlying idea is to separate current injection and voltage sensing probes to eliminate the influence of distorting contact resistances. Among others, the technique is commonly utilized in multi-tip scanning tunneling microscopy setups (see e.g. [1]). The necessity to perform both voltage and current measurements, however, requires either impracticable rewiring in between measurements or complex electronics, which can perform both measurements but are prone to induce additional electrical noise. By using current sensing probes to measure the voltage via a feedback loop [2] we introduce a new approach that allows to conduct low noise and in principle truly non-invasive four-point probe measurement at the nanometer scale.

[1] S. Just, M. Blab, S. Korte, V. Cherepanov, H. Soltner, and B. Voigtländer, Phys. Rev. Lett. 115, 066801 (2015)

[2] F. Lüpke, S. Korte, V. Cherepanov, and B. Voigtländer, Rev. Sci. Instr. 86, 123701 (2015)

O 80.7 Wed 18:15 Poster A

Detection of spin-polarized transport in topological insulators using a 4-tip STM — •Arthur Leis, Sven Just, Vasily Cherepanov, and Bert Voigtländer — Peter Grünberg Institut (PGI-3) and JARA-FIT, Forschungszentrum Jülich, Germany

Spin-momentum locked surface states as a hallmark of topological insulators are of particular interest in solid-state physics. However, the detection of these states in transport measurements is a challenge, as a spin-sensitive measurement technique is needed. While most measurement efforts are based on optical methods, reports on the electrical detection of spin-polarized charge transport are still scarce and include lithographic sample preparation. Our approach to this challenge is an in-situ distance-dependent four-point probe measurement technique using a multi-tip STM with magnetic tips. While distance-dependent measurements are used for the distinction between 2D- and 3D-transport, using magnetic tips allows for the detection of spin-polarization.

O 80.8 Wed 18:15 Poster A

STM with fibre tips : A new approach to probe the local optical response of surfaces — •René Jakob and Niklas Nilius — Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany

STM is an ideal tool to measure topographic and electronic properties of surfaces at atomic length scales. STM luminesce spectroscopy, which uses the inelastic tunnelling current to stimulate photon emission, enables a local optical characterization in addition. Main drawback is the low coupling strength of electrons and photons in the tip-sample gap, yielding reasonable signal-to-noise ratios only if using plasmonic materials for tip and sample. We have attempted to overcome this difficulty by coupling laser light directly into the STM junction via an optical fibre tip. To activate also the tunnelling channel, the fibre tip is coated with layers of Cr/Ag or Cr/Au. The interaction of incident photons with the surface is measured via a CCD detector in the far-field. The approach allows us to probe the optical response of surfaces covered with molecules, metal particles or oxide colour centres with high spatial resolution.

O 80.9 Wed 18:15 Poster A

Analysis of CO-terminated tips used by combined STM/AFM at low temperatures — •Julian Berwanger, Ferdinand Huber, and Franz J. Giessibl — University of Regensburg, 93040 Regensburg, Germany

The functionalization of scanning probe microscope tips with a carbon monoxide molecule - introduced by Bartels et al. [1] for STM and by Gross et al. [2] for AFM - is widely used today due to their atomic resolution capability on molecules, metallic clusters and other sample systems [2-4]. The exact imaging mechanism and the influence of bending effects of the CO tip on experimental data was studied extensively [5-8]. Nonetheless a study which explains that various CO-terminated tips can lead to different qualitative and quantitative results, especially in the short range interaction regime, is - to our knowledge - missing. We analyze AFM data of single metal adatoms on Cu(111) imaged by CO-terminated metal tips with various opening angles and present a hypothesis about the observed difference in the experimental contrast of single adatoms.

[1] L. Bartels et al. Appl. Phy. Lett. 71, 2 (1997)
[2] L. Gross et al. Science 325, 110 (2009)
[3] M. Emmrich et al. Science 348, 6232 (2015)
[4] M. Ellner et al. Nano Lett. 16, 3 (2016)
[5] M. Neu et al. PRB 89, 205407 (2014)
[6] N. Moll et al. New J. Phys. 12, 125020 (2010)
[7] P. Hapala et al. PRB 90, 085421 (2014)
[8] P. Hapala et al. Nat. Com. 7, 11560 (2016)

O 80.10 Wed 18:15 Poster A

Practical considerations in 3D magnetic resonance force microscopy — •Marc-Dominik Krass, Urs Grob, Alexander Eichler, Martin Héritier, Hiroki Takahashi, and Christian Degen — Department of Physics, ETH Zurich, Otto-Stern-Weg 1, 8093 Zurich, Switzerland

Magnetic resonance force microscopy (MRFM) is a technique that reconstructs the 3D density distribution of nuclear spin species in nanoscale samples, such as individual macromolecules. While the feasibility of the method has been demonstrated [Degen et al. PNAS 106, 1313 (2009)], state-of-the-art experiments have not yet reached the subnanometer regime required to reveal detailed molecular structures.

MRFM experiments operate at the physical boundaries of technology where every improvement in resolution must be earned by overcoming a manifold of physical and technical problems. Of crucial importance are, for instance, a stable feedback control of the mechanical resonator, a superb displacement detection sensitivity, suppression of standing waves in the rf-circuit and clever NMR pulse shaping for evading unwanted electrostatic interaction, and robust spin inversion protocols. Our poster summarizes our progress in MRFM technology and demonstrates first signal scans of single isotope-labeled influenza virus particles.

O 80.11 Wed 18:15 Poster A

Measuring Single Iron Magnetic State Lifetimes Using Distortion Compensated Signals — •Gregory McMurtrie[1,2,3], Max Hänze[2,3], Steffen Rolf-Pissarczyk[2,3], Luigi Malavolti[2,3], Mohammad Abdo[2,3], Björn Schlie[1,2,3], and Sebastian Loth[1,2,3] — [1]Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Structure and Dynamics of Matter, Hamburg, Germany — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany

Injecting pulses [1] or continuous wave signals [2] into a tunnel junction has shown promising results for the characterization of fast magnetic surface dynamics using scanning tunneling microscopy. When pushing into the sub-nanosecond time domain, the transmission line characteristics of the instrument strongly modify the signals reaching the tunnel junction [3], limiting the effective time resolution. We present an in-situ technique for the quantitative measurement of the transmission line characteristics, both in phase and amplitude. This information is used to compensate for imperfections in the transmission lines, resulting in a greatly increased effective bandwidth. By improving the time resolution of the instrument, it becomes possible to measure spin relaxation times of individual atoms which are often well under a nanosecond. The door is now opened to further implement the pulse correction technique and observe a wide range of ultra-fast phenomena at the atomic scale. [1] S. Loth, et. al. Science 329 1628 (2010). [2] S. Baumann et. al. Science 350 6259 (2015) [3] C. Grosse, et. al. Appl. Phys. Lett. (2013)

O 80.12 Wed 18:15 Poster A

Design of a 30 mK scanning tunneling microscope for spin-polarized measurements — •Sebastian Schimmel, Danny Baumann, Alexander Horst, Ralf Voigtländer, Dirk Lindackers, Bernd Büchner, and Christian Hess — IFW Dresden, Helmholtzstrasse 20, 01069, Dresden, Germany

In order to obtain experimental access and to disentangle the intertwined phases found in unconventional superconductors, which are namely the electronic ordering, superconductivity and static magnetism, we designed the presented milli-Kelvin scanning tunneling microscope (STM) system for spin-polarized investigation with very high resolution in energy as well as in real space. Using a 3He/4He Dilution Refrigerator allows to cool the tip and sample to a measurement temperature of 30 mK that improves the energy resolution to the corresponding value of only about 15 micro-eV and enables to study all classes of unconventional superconductors, also including heavy fermion compounds. Long term measurements at base temperature can be performed for up to 7 days. A 9-4 T vector magnet allows the systematic in-situ manipulation of the spin-polarization axis. For the preparation of tips and samples for spin-polarized STM measurements, a UHV chamber has been designed with a suitable system for tip/sample transfer. The suppression of disruptive vibrations is done by a two stage passive/active damping system.

O 80.13 Wed 18:15 Poster A

Tests and first results of an RF-compatible UHV-based multiprobe-STM system — •Jonas Koch, Jonas Harm, Johannes Friedlein, Maciej Barzanik, Stefan Krause, and Roland Wiesendanger — Dept. of Physics, University of Hamburg, Hamburg, Germany

We present the concept of a 3-tip multiprobe scanning tunneling microscope (MP-STM), which achieves picosecond time resolution by the use of RF technology. The evaluation of the microscope's performance is carried out in ultra-high vacuum (UHV) and at variable temperatures from 30 K up to room temperature. For this purpose we have designed a vibration-damped UHV setup equipped with electrical RF feedthroughs (for up to 40 GHz). The tests focus on the thermal coupling of individual components, in particular the RF cabling, and on the vibration decoupling from external noise sources. Furthermore, we analyzed the behavior of the coarse drive in x-, y- and z-direction for each of the three scanners at low temperatures. First results of the 3-tip multiprobe-STM will be presented.

O 80.14 Wed 18:15 Poster A

GXSM3: an open source scanning probe system — Percy Zahl[1], •Thorsten Wagner[2], and GXSM community[3] — [1]Center for Functional Nanomaterials, Brookhaven National Laboratory, USA — [2]Experimental Physics, Johannes Kepler University, Linz, Austria — [3]gxsm.sf.net and sranger.sf.net

Pushing the limits of scanning probe microscopy (SPM) does not only require a dedicated hardware (microscope) but also a sophisticated control system. In particular, the open source and community driven project GXSM [1-3] provides a high level of flexibility so that different kinds of SPMs can be operated via a digital signal processor (DSP) based hardware. Recently, the third version of the graphical user interface was released. Besides the completely overhauled user interface based on the Gtk+3/Gnome3-standard, there are also significant changes under the hood: The possibilities to remotely control GXSM3 via Python scripts were widely extended. Complex data acquisition tasks like automatic mosaic/survey scans are easily programmed in a simple script. Even auto-approach schemes with 'watch dog'-option for the frequency (AFM mode) can be put into action by Python scripting. Tip position can now be controlled via mouse/objects and is fully programmable via python. A new open GL based 3D view was implemented, which allows also the rendering of volumetric data. Now, several wave forms can be used for the coarse motion.

[1] P. Zahl *et al.*, Imaging & Microscopy (GIT), Jan. 26, 2015.
[2] P. Zahl, *et al.*, J. Vac. Sci. Technol. B 28 (2010) C4E39.
[3] P. Zahl, *et al.*, Rev. Sci. Instr. 74 (2003) 1222.

O 80.15 Wed 18:15 Poster A

An STM in a Pulse-Tube Refrigerator — •Marcel Rost, Gert Koning, Ko Koning, and Tjerk Oosterkamp — Huygens-Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

The advantage of Pulse-Tube Refrigerators over conventional (wet) ones becomes obvious, if one considers the (future) increase in helium costs as well as the complexity, maintenance, and time investment that is required to run a wet-type refrigerator. However, the clear downside of a pulse-tube-system is the acoustical and mechanical noise introduced by the pulsing pump.

Although we have successfully shown earlier that it is possible to obtain atomic resolution on HOPG with an STM in our system, the real demonstration, however, is obtaining at least full atomic resolution on a closed packed fcc(111) surface! Here we show our current approach, the modifications of the STM, and present the latest results.

O 80.16 Wed 18:15 Poster A

Modelling force sensor oscillations for non-contact atomic force microscopy — •Daniel Heile, Philipp Rahe, and Michael Reichling — Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück

The force sensors utilized in non-contact atomic force microscopy are prevalently described by the Euler-Bernoulli beam equation which is commonly analytically solved in the load free, homogeneous case. Furthermore we consider cases, where this analytical approach is not viable any more and introduce the finite differences method (FDM) to describe the force sensor oscillation and dynamics. FDM allows the description of the cantilever oscillations as an eigenvalue problem based on the Euler-Bernoulli beam equation. The results of both approaches are compared for several fundamental cases verifying the reliability of the FDM for force sensor modelling. Based on these results more advanced models, for example coated force sensors, can be considered.

O 80.17 Wed 18:15 Poster A

Coupling microwave radiation into an STM Josephson junction — •Nils Bogdanoff[1], Olof Peters[1], Gaël Reecht[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Univ. Grenoble Alpes, Institut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

Josephson junctions (JJ) have been extensively studied as promising elements in quantum mechanical circuits. Combining them with the high spatial resolution of a scanning tunneling microscope (STM) would allow for the local investigation of the superconducting groundstate close to magnetic defects. We present a current-biased JJ formed between Pb tip and Pb sample in a $T = 1.3\,\mathrm{K}$ STM.

Microwave frequencies of up to $f = 26\,\mathrm{GHz}$ can be introduced into the junction using coaxial cables. The Josephson current responds to the irradiation by showing multiple frequency- and power-dependent steps. Simulations allow to distinguish their origin between coherent and incoherent as well as Cooper pair- and quasiparticle-based processes.

O 80.18 Wed 18:15 Poster A

Development of an ultrafast THz-gated Scanning tunneling microscope combined with optical photoexcitation — •Natalia Martín Sabanés, Mellanie Müller, and Martin Wolf — Fritz Haber Institute, Berlin, Germany

Unravelling the complex spatio-temporal dynamics of nanostructures and molecules is essential to optimize a variety of applications in nanoelectronics or energy conversion devices. Focusing THz-pulses into the junction of a scanning tunneling microscope (STM) modulates the bias on ps to fs time scales, providing ultrafast control of the tunneling current. THz-gated STM has been successfully used to monitor ultrafast processes on atomic length scales employing a THz pump-THz probe excitation scheme.[1] Despite the outstanding capabilities that this scheme holds for the study of ultrafast phenomena on the atomic level, different experimental configurations allowing the use of optical photoexcitation remain unexplored. We introduce the technical development of an ambient THz-gated STM combined with near-field optical photoexcitation. We discuss the suitability of different THz emitters as well as the use of plasmonic nanofocusing on nanostructured gold tips to increase photoexcitation efficiency and to reduce the thermal load of the tunneling junction.[2] Combining the atomic spatial and fs temporal resolution of a THz-gated STM with optical photoexcitation will provide access to a broader range of spatio-temporal phenomena.

[1] Nature Photonics, 2013, 7(8), 620-625. Nature,2016 539(7628), 263-267. Nature Physics, 2017, 13(6), 591-598. [2] ACS Photonics, 2016, 3(4), 611-619.

O 80.19 Wed 18:15 Poster A

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

To realize the vision of molecular electronics, the precise control of molecular conformations is critical. The scanning probe microscope (SPM) is the tool of choice for the controlled manipulation of single molecules on surfaces. Finding the right manipulation protocol for a given task can be complicated due to the large number of degrees of freedom of such systems. The computationally demanding search for correct manipulation trajectories via simulation can be avoided if a clear manipulation goal can be formulated. In this case the experimenter can *learn* to achieve this goal in a trial and error approach [1,2]. Here we go one step further and delegate the learning process to a computer. We use reinforcement learning to train a neural network for the task of removing individual PTCDA (3,4,9,10-perylenetetracarboxylicdianhydride) molecules from a monolayer on Ag(111). The feasibility of our approach is proven using simulated manipulation and first steps are shown of how to employ the method in an experimental SPM setup. [1] M. F. B. Green et al. Beilstein J. Nanotechnol. 5, 1926 (2014) [2] P. Leinen et al. J. Vis. Exp. (116), e54506 (2016)

O 80.20 Wed 18:15 Poster A

Towards a radio frequency four tip scanning tunneling microscope — •Jonas Duffhauss[1], Marco Pratzer[1], Vasily Cherepanov[2], Bert Voigtländer[2], and Markus Morgenstern[1] — [1]RWTH Aachen University/JARA-Fit — [2]Jülich Research Center

A four tip STM [1] has been modified with different cablings that allow for STM measurements in the GHz regime. The time resolution has been determined by a pump-probe experiment using a sample with a non-linear $\mathrm{d}I/\mathrm{d}V$ characteristic (Gold, HOPG) [2].

A time resolution of $< 180\,\mathrm{ps}$ was demonstrated if a RF-cable is used as tip, which is likely limited by the voltage pulse generator. Using the four tip STM with the already implemented tip exchange mechanism, the time resolution gets worse ($\approx 350\,\mathrm{ps}$) due to the additional impedance missmatch. Ringing effects caused by standing waves inside the cable and a low transmission at high frequencies (10 GHz) are identified as main cause for the reduced time resolution.

Options for further improvements of the RF parts, e.g., a low noise bias-tee, are discussed.

[1] V. Cherepanov, E. Zubkov, H. Junker, S. Korte, M. Blab, P. Coenen, and B. Voigtländer, Rev. Sci. Instr., 83, 033707 (2012).

[2] C. Saunus, J. R. Bindel, M. Pratzer, and M. Morgenstern, Appl. Phys. Lett. 102, 051601 (2013).

O 81: Poster Focus Session: Molecular Nanostructures on Surfaces - New Concepts towards Complex Architectures

Time: Wednesday 18:15–20:30 Location: Poster A

O 81.1 Wed 18:15 Poster A

On-Surface Metalation of Corrole Ligands — •Jan Herritsch, Malte Zugermeier, Min Chen, Qitang Fan, Martin Schmid, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

The surface coordination chemistry of porphyrinoid transition metal complexes plays an important role in interface functionalization. Variation of the ligand skeletal structure offers the possibility to tune and control the reactivity. Corroles can be described as contracted porphyrins, which however differ in their electronic structure and can act as formally trianionic ligands. We have studied the characteristics of mono- and submonolayers of a free-base alkyl substituted corrole ligand system on the Ag(111) and the Cu(111) surface. Furthermore, we present two different ways for the on-surface syntheses of transition metal corrole complexes. On the one hand we were able to show the synthesis of cobalt corrole on the Ag(111) surface through metalation of a ligand monolayer by postdeposition of the corresponding metal. As a second route we studied the thermally controlled self-metalation of corrole with substrate atoms on the Cu(111) surface yielding a copper corrole complex. The reactions were investigated by XPS, UPS and STM studies and compared to a similar porphyrin as a reference system. DFT calculations were performed to obtain additional insight and to interpret the spectra.

O 81.2 Wed 18:15 Poster A

Growth and Electronic Properties of a Potential Organic Su-

perconductor on Cu(111) — •Felix Otto, Bernd Schröter, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Several polycyclic aromatic hydrocarbons (PAHs) become superconducting after the intercalation of alkali metal atoms. The number of promising candidates has increased in the last few years. Among them, $K_{3.45}$1,2:8,9-dibenzopentacene (trans-DBPen, $C_{30}H_{18}$) is the one with the highest critical temperature of 33.1 K reported so far [1]. Nevertheless, the microscopic mechanisms of superconductivity in K-doped PAHs are still under debate. One open question is, for example, the effect of structural order in bulk materials as well as two-dimensional layers.

Our work deals with the growth of trans-DBPen on Cu(111) in the monolayer (ML) regime. The self-assembled thin films were prepared using organic molecular beam epitaxy. The structure was characterized by means of low energy electron diffraction (LEED). X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS) were used to study the interaction of the molecules with the substrate. In the sub-ML range we observe a 2D gas-like behavior, whereas the first ML is characterized by a highly ordered structure. The results are compared to measurements of trans-DBPen on Au(111) and Ag(111) in terms of the molecule-substrate interaction.

[1] M. Xue *et al.*, Sci. Rep. **2**, 389 (2012).

O 81.3 Wed 18:15 Poster A

Bilayer Formation vs. Monolayer Replacement in Organic Heterostructures: Strong Impact of Subtle Changes in Molecular Structure — •Qi Wang[1,2], Antoni Franco-Canellas[2], Penghui Ji[1], Haiming Zhang[1], Alexander Gerlach[2], Lifeng Chi[1], Steffen Duhm[1], and Frank Schreiber[2] — [1]Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, China — [2]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany

The electronic structure at the interfaces of copper-phthalocyanine (CuPc) on 6,13-pentacenequinone (P2O) or 5,7,12,14-pentaceneterone (P4O) pre-covered Ag(111) was investigated using ultraviolet photoelectron spectroscopy (UPS), X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM). Despite the similar chemical structure of P2O and P4O, their monolayers on Ag(111) are strikingly different: while P2O is physisorbed, P4O is strongly chemisorbed involving a net electron transfer from the substrate to the adsorbate.[1] Similarly, also CuPc interacts heavily with Ag(111)[2] leading to chemical core-level shifts. By combining our UPS, XPS and STM results for mono- and heterostructures we obtain a full picture of interface energetics and can disentangle competing intermolecular and adsorbatesubstrate interactions.

[1] G. Heimel, et.al. Nat. Chem. 2013, 5, 187.

[2] I. Kröger, et.al. New J. Phys. 2010, 12, 083038.

O 81.4 Wed 18:15 Poster A

Reversible switching of azobenzene tetramers molecules at a metal surface — •christophe nacci[1], massimo baroncini[2], alberto credi[2], and leonhard grill[1] — [1]Department of Physical Chemistry, University of Graz, 8010 Graz, Austria — [2]Photochemical Nanosciences Laboratory, University of Bologna, 40126 Bologna, Italy

Molecular switches revealing reversible isomerization properties are potentially relevant building blocks in the fields of molecular electronics, functionalized surfaces and information storage. Azobenzene is a prototypical molecular switch owing to the trans-cis isomerization of the central double nitrogen bond. Here, we report a study on azobenzene tetramers which are comprised of four azobenzene units in a tetrahedral arrangement. By using low-temperature scanning tunneling microscopy and spectroscopy (STM/STS) we can image individual molecules and study their switching properties with high spatial resolution. After adsorption on a Ag(111) surface we find molecular aggregates with characteristic hexagonal shapes that can be assigned to periodic adsorption sites. Reversible isomerization of azobenzene tetramer molecules was then induced either by the microscope tip or laser illumination. By analyzing the switching behavior, we obtain insight into the coupling with the surface and the effect on the physical/chemical properties of the molecules.

O 81.5 Wed 18:15 Poster A

Coverage dependent self-assembly structures of Co (II) 5, 15-diphenylporphyrin on Cu (111) — •Feifei Xiang, Anja Gemeinhardt, and M. Alexander Schneider — Solid State Physics, Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Erlangen, Germany

The self-assembly structure of Co (II) 5,15-diphenylporphyrin (Co-DPP) on Cu (111) as a function of molecular coverage is studied and compared with unmetalated 5,15-diphenylporphyrin (2H-DPP) by low temperature scanning tunneling microscopy. Both 2H-DPP and Co-DPP show chirality on the copper surface due to the distortion of the molecular skeleton. 2H-DPP can only form chain-like, 1D structures on the surface. The self-assembly structure of Co-DPP varies from low molecular coverage to very dense coverage. At very low molecular coverage, the Co-DPP forms triangular structures and 1-D chains, which follow the 3-fold symmetry of the substrate. When the molecular coverage is higher than half monolayer, Co-DPP forms square and rectangular 2D networks caused by the chirality of the molecular configurations. At full monolayer coverage the molecules are closely packed in a racemic mixture.

O 81.6 Wed 18:15 Poster A

Supramolecular networks of arylene-alkynylenes on HOPG: STM studies — •Tristan J. Keller, Georgiy Poluektov, Stefan-S. Jester, and Sigurd Höger — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Straße 1, 53121 Bonn, Germany

We report about the synthesis and 2D supramolecular self-assembly of shape persistent arylene-alkynylene macrocycles at the solid/liquid interface on HOPG. The molecules form complex supramolecular architectures that ar imaged by scanning tunneling microscopy with submolecular resolution. The flexible alkyl/alkoxy side chains interdigitate intermolecularly and stabilize the network formation. The investigation aims at detailed understanding on how the pattern structures and lattice constants depend on the exact shape of the backbones as an effect of the respective corner units and the strain induced by them. In addition, the role of experimental parameters (concentration, thermal annealing) is investigated. [1] P. Wilhelm, J. Vogelsang, G. Poluektov, N. Schönefelder, T. J. Keller, S.-S. Jester, S. Höger, J. M. Lupton, *Angew. Chem. Int. Ed.* **2017**, *56*, 1234-1238.

O 81.7 Wed 18:15 Poster A

Resolving intramolecular-distortion changes induced by the partial fluorination of pentacene adsorbed on Cu(111) — •Antoni Franco-Cañellas[1], Qi Wang[1,2], Katharina Broch[1], Bin Shen[2], Alexander Gerlach[1], Holger F. Bettinger[2], Steffen Duhm[3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Institut für Organische Chemie, Universität Tübingen, Germany — [3]Institute of Functional Nano & Soft Materials (FUNSOM) and Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Soochow University, People's Republic of China

We experimentally quantify the molecular bending of the partially-fluorinated pentacene (PEN) compound 2,3,9,10-tetrafluoropentacene (F4PEN) adsorbed on Cu(111). By means of the X-ray standing wave (XSW) technique, we directly measure the adsorption distance of three inequivalent carbon species, the fluorine atoms, as well as the total and backbone carbon average adsorption distances. This allows us to resolve two adsorption behaviors, namely, a PEN-like strong coupling between the backbone and the substrate and a repulsive interaction involving the fluorinated short molecular edges, which are 0.9 Å above the central benzene ring. This finding is further supported by additional ultraviolet photoelectron spectroscopy and low-energy electron diffraction measurements, thus showing that the selective fluorination of a PEN molecule has only a local conformational effect and it is not enough to modify its interface properties.

O 81.8 Wed 18:15 Poster A

One-dimensional molecular chains of Quinacridone on Ag(100) and Cu(111): STM- and SPA-LEED-investigations — •Niklas Humberg, Alexander Eslam, and Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany

We report a structural analysis of Quinacridone (QA) on Ag(100) and Cu(111) by scanning tunneling microscopy (STM) and spot profile analysis low energy electron diffraction (SPA-LEED). On Ag(100) QA grows at room temperature in parallel homochiral one-dimensional chains, forming a metastable structure. Within these chains the molecules are closely packed and linked via hydrogen bonds. The distance between two neighboring chains varies with coverage. After annealing to 500 K a commensurate heterochiral structure is formed. It consists of homochiral dimers forming periodically idented chains. An oblique unit cell with cell parameters $a = (14.3 \pm 0.3)$ Å, $b = (16.9 \pm 0.3)$ Å and $\alpha = (112 \pm 0.5)°$ was found.

SPA-LEED patterns of QA on Cu(111) suggest the presence of more disorder. The observed spots smear out, creating a highly symmetric diffraction pattern containing many lines with varying intensities.

O 81.9 Wed 18:15 Poster A

Synthesis of different experimental techniques in surface science: DBP films on graphitic sufaces — •Tino Kirchhuebel[1], Fabio Bussolotti[2], Jinpeng Yang[4], Keiichirou Yonezawa[2], Ryo Shiraishi[2], Takuma Yamaguchi[2], Taka Ueba[2], Ryosuke Mori[3], Shogo Kunieda[3], Takashi Yamada[3], Tobias Huempfner[1], Roman Forker[1], Toshiaki Munakata[3], Satoshi Kera[2,4], and Torsten Fritz[1] — [1]FSU Jena, Germany — [2]IMS Okazaki, Japan — [3]Osaka University, Japan — [4]Chiba University, Japan

We present a comprehensive study on highly ordered thin films of the lander molecule tetraphenyldibenzoperiflanthene grown on graphitic surfaces. The spectra from ultraviolet photoelectron spectroscopy (UPS) combined with inverse photoelectron spectroscopy (IPES), two-photon-photoemission (2PPE), and optical spectroscopy (DRS) are discussed in context with the film structure, investigated with scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). The interpretation of different spectroscopic data is a challenging task. Here, the comparison reveals seeming discrepancies regarding the coverage dependent energy level alignment of DBP films. Facing this problem, a model based on charging and polarization effects is introduced, which explains the observations consistently.

O 81.10 Wed 18:15 Poster A

Determination of critical cluster size, diffusion barrier and cohesion energy of PTCDA on Cu(001) — •Janina Felter, Jana Wolters, Markus Franke, Gerben van Straaten, Caroline Henneke, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, 52425 Jülich, Germany

Understanding the adsorption and growth mechanisms of large π-conjugated molecules on noble metals is a key issue for designing and optimizing organic electronic devices. Here, we report on the growth of PTCDA on Cu(001) studied in situ and in real time with Low-Energy Electron Microscopy (LEEM). By analysing island size distributions within the aggregation regime and applying methods developed for atomic nucleation on surfaces, we were able to determine the critical cluster size i for the formation of stable clusters for temperatures between 300 K and 390 K. We find different values (i = 1 and i = 3) for two different temperature regimes. This allows us to determine the diffusion barrier for individual molecules and, with the help of pair-potential calculations, the cohesion energy of a cluster of two molecules.

O 81.11 Wed 18:15 Poster A

Fluorescence microscopic analysis on the orientation of PTCDA domains on KCl(100) in ultrahigh vacuum — •Nils Rohbohm[1], Christian Marquardt[1], Rudolf Merkel[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany — [2]Institute of Complex Systems, ICS-7: Biomechanics, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

We report data obtained by an epi-fluorescence light microscope directly attached to a surface science UHV-chamber. We have studied the fluorescent and superradiant domains formed in the monolayer of PTCDA on a thin epitaxial film of KCl on a Ag(100) surface. The domains exhibit a brick-wall-type structure and nucleate in two perpendicular orientations. Using additional rotatable polarisation filters in the incident and detected beam paths, we can spatially discriminate the two types of differently oriented domains. At present the spatial size of one domain can be as large as 1000 μm^2. From the microscopic images we deduce information on the domain growth in relation to the local surface morphology. Brightfield images of the underlying Ag(100) surface show a macroscopic corrugation which appear to be correlated with the pattern of the PTCDA domains detected by fluorescence. Supported by the DFG.

O 81.12 Wed 18:15 Poster A

Adsorption Conformation and Lateral Registry of Cobalt Porphines on Cu(111) — Martin Schwarz[1], Manuela Garnica[1], David Duncan[2], Alejandro Perez Paz[3], Jacob Ducke[1], Peter Deimel[1], Pardeep Kumar Thakur[2], Tien-Lin Lee[2], Angel Rubio[4], Johannes V. Barth[1], Francesco Allegretti[1], and •Willi Auwärter[1] — [1]Technische Universität München, Germany — [2]Diamond Light Source, United Kingdom — [3]Yachay Tech University, Ecuador — [4]Max-Planck-Institut für Struktur und Dynamik der Materie, Germany

The tetrapyrrole macrocycle of porphine is the common core of all porphyrin molecules, an interesting class of π-conjugated molecules with relevance in natural and artificial systems [1]. The functionality of porphines on a solid surface can be tailored by the central metal atom and its interaction with the substrate [2]. Here, we present a local adsorption geometry determination for cobalt porphine on Cu(111) by means of complementary scanning tunneling microscopy, high-resolution X-ray photoelectron spectroscopy and X-ray standing wave measurements, and density functional theory calculations. Specifically, the Co center was determined to be at an adsorption height of 2.25 ± 0.04 Å occupying a bridge site. The macrocycle adopts a moderate asymmetric saddle-shape conformation. Based on these results, we will discuss the interfacial interactions for this archetypical metallotetrapyrrole/metal system.

[1] F. Bischoff et al., ACS Nano 7, 3139 (2013)

[2] K. Diller et al., Chem. Soc. Rev. 45, 1629 (2016)

O 81.13 Wed 18:15 Poster A

Tuning the band structures of graphene nanoribbons by functionalized edge groups — •Jingcheng Li[1,2], Néstor Merino-Díez[2,3], Eduard Carbonell-Sanroma[1], Jeremy Hieulle[1], Manuel Vilas-Varela[5], Aran García-Lekue[3], Pedro Brandimarte[2], Martina Corso[2,4], Daniel Sanchez-Portal[2], Dimas G. de Oteyza[3,4], Aitor Mugarza[6], Diego Peña[5], and Jose Ignacio Pascual[1,4] — [1]CIC Nanogune, 20018 San Sebastián, Spain — [2]CFM, 20018 San Sebastián, Spain — [3]DIPC, 20018 San Sebastián, Spain — [4]Ikerbasque, 48013 Bilbao, Spain — [5]CIQUS, 15782 Santiago de Compostela, Spain — [6]ICN2, 08193 Barcelona, Spain

On-surface synthesis of atomically precise graphene nanoribbons (GNRs) allows engineering the band structures of GNRs by modifying the molecular precursors. Until now, most of the works are focused on the chemical substitution of carbon atoms by heteroatoms in GNRs. Here in this work, we show that band structure of GNRs can be tuned by edge functionalization of GNRs. The effect of cyano (-CN) edge group on the band structure of armchair GNRs (aGNRs), and the effect of amino (-NH2) and nitro (-NO2) edge groups on the band structure of chiral GNRs (cGNRs) are studied. We found that cyano edge groups act as n-dopants, down-shifting the bands of aGNRs, while amino edge groups acts as p-dopants, up-shifting the bands of cGNRs. Due to the reactivity of nitro edge groups on surface, their effect on the band structures of cGNRs need to be further clarified.

O 81.14 Wed 18:15 Poster A

Adsorption of Porphyrin on Cu (111) - Chemisorption and physisorption — •Konstantinos Koumpouras, Jakub Baran, and Andreas J. Larsson — Applied Physics, Division of Materials Science, Department of Engineering Sciences and Mathematics, Lulea University of Technology, SE-971 87 Lulea, Sweden

In recent years, the investigation of porphyrin molecules on surfaces is of great interest due to their potential applications in several fields. The main characteristics which make them suitable candidates in these fields are that they possess an impressive variety of functional properties and are extraordinary stable. Since one research part of the porphyrins is focused on their use as elements for future molecular electronic systems, the interaction between them and solid surfaces is very important. The main advantage is the preservation of gas-phase flexibility during their deposition on metal surfaces where a number of distinct conformers are observed.

The Cu (111) surface is widely used as the adsorption "platform" for studying the different conformation of porphyrin molecules where the interactions are dominated by chemical interactions or attractive van der Waals interactions or both. Conformational changes due to the adsorption of the molecule can affect its properties but the mechanisms that drive these changes are often unclear, so detailed studies of different molecule - surface interactions by means of density functional theory is more than necessary for a comprehensive analysis and interpretation of experimental data.

O 81.15 Wed 18:15 Poster A

Self-assembly of cyano-substituted porphyrin-derivatives on bulk insulators — •Min-Ken Li, Jia Liu, Mirunalini Devarajulu, and Sabine Maier — Department of Physics, Universität Erlangen-Nürnberg, Erlangen, Germany

The realization of molecule-based devices requires functional molecular building blocks integrated on suitable substrates. Due to the strong interaction between molecular building blocks and metal surfaces, most molecules lost their original functionality on metal surfaces. The weak interaction between organic molecular building blocks and bulk insulating surfaces makes it ideal for the fabrication of molecular devices. Hence, organic molecules adsorbed on insulating surfaces have been attracting more and more attention recently.[1] Here, we present a study on the self-assembly of cyano-substituted tetraphenylporphyrin derivatives on bulk KBr(001) and MgO(0001) by non-contact atomic force microscopy (AFM) at low temperature. We observed two-dimensional self-assembly of the cyano-substituted tetraphenylporphyrin derivatives. The interaction between intermolecular cyano and phenyl groups plays an essential role in the formation of the 2D self-assembly.[2] The structure of the self-assembly will be discussed in detail based on AFM images featuring sub-molecular resolution.

[1] P. Rahe, et al. Advanced Materials, 2013, 25-29, 3948-3956
[2] S. Maier, et al. Small, 2008, 4, 1115-1118

O 81.16 Wed 18:15 Poster A

On-surface self-assembly of tetratopic molecules with directional interactions: insights from computer modeling — •Damian Nieckarz[1], Paweł Szabelski[1], and Wojciech Rzysko[2] — [1]Department of Theoretical Chemistry, Maria Curie-Skłodowska University, Lublin, Poland — [2]Department for the Modeling of Physico-Chemical Processes, Maria Curie-Skłodowska University, Lublin, Poland

The Monte Carlo simulation method was used to explore structure formation in adsorbed assemblies comprising tetratopic molecules equipped with active terminal arm segments. Depending on the interaction directions assigned to the active sites, the simulations resulted in the formation of extended ordered, chain-like and glassy structures. In several cases, complex porous patterns have been observed, especially when polymorphic phases were formed. Our calculations demonstrated that the tetratopic building blocks can undergo spontaneous self-assembly to produce a wide range of molecular superstructures with tunable properties like, for example, nanopore shape and size, chirality and periodicity. These theoretical predictions may be helpful in experimental construction of new molecular architectures with precisely defined morphologies and functionalities using the bottom-up approach.

The financial support of the Polish National Science Centre (grant 2015/17/B/ST4/03616) is gratefully acknowledged

O 81.17 Wed 18:15 Poster A

Effects of neutron irradiation on the frequency dependencies of electrical conductivity of nanocrystalline 3C-SiC particles — •Elchin Huseynov — Institute of Radiation Problems of Azerbaijan National Academy of Sciences, AZ 1143, B.Vahabzade 9, Baku, Azerbaijan

Nanocrystalline 3C-SiC have been irradiated by neutron flux up to 20 hours. On the 3C-SiC nanomaterial radiation-induced conductivity (RIC) has been observed after neutron irradiation. From the comparatively analyses of frequency dependence of electrical conductivity at different temperatures it was determined that, numerical value of electrical conductivity increases after neutron irradiation. Numerical value of electrical conductivity of 3C-SiC nanomaterial increases up to 7.5x10-4 S/m or approximately 5.5 times after neutron irradiation. The main reason for RIC is the increase of concentration of carriers in nanocrystalline 3C-SiC after neutron irradiation. It has been determined from interdependence between real and imaginary parts of electrical conductivity that, the real part of electrical conductivity changes more than imaginary part after neutron irradiation. Ionic or dipolar type of conductivity has been found from interdependence between real and imaginary parts of electrical conductivity. Moreover, acceptor or donor defects are known as deep levels are generated in nanomaterial after neutron irradiation. The concentration of donor (n-type donor, 31P) atoms increases as a result of nuclear transformation within neutron irradiation in 3C-SiC nanomaterial and it is one of the factors leading to increase of conductivity.

O 81.18 Wed 18:15 Poster A

DHTAP thin layers deposited on Cu(110) and Cu(110)-(2×1)O surfaces — •Andrea Navarro-Quezada[1,2], Michael Györök[2], Thorsten Wagner[2], Anthony Thomas[3], Thomas Leoni[3], Alain Ranguis[3], Conrad Becker[3], and Peter Zeppenfeld[2] — [1]Solid State and Semiconductor Physics, JKU Linz, Austria — [2]Experimental Physics, JKU Linz, Austria — [3]CINAM, Marseille, France

Dihydrotetraazapentacene (DHTAP) is a derivate of pentacene, which due to its two H-donor (N-H) and the two H-acceptor (N=C) sites, is expected to form well-ordered molecular structures on surfaces. Here, we study the morphology and the evolution of the optical properties during the deposition of DHTAP thin layers on Cu(110) and Cu(110)-(2×1)O surfaces using polarization-dependent differential reflectance spectroscopy (pol-DRS)[1] in combination with photoelectron emission microscopy (PEEM). We compare our results to those obtained by in situ reflectance differential spectroscopy (RDS) in a second experiment. Within the first monolayer, DHTAP absorbes in a flat-lying geometry on both surfaces. However, the orientation of the long molecular axis of the molecules in the first monolayer is aligned along the [1-10]-direction on the Cu(110) surface, while it is parallel to the [001]-direction on Cu(110)-(2x1)O. We find that, depending on the growth temperature, the DHTAP molecules on top of the first monolayer deposited on Cu(110) change their preferential alignment.

[1] A. Navarro-Quezada *et al.*, Rev. Sci. Instr. 86, 113108 (2015)

O 82: Poster Focus Session: Frontiers of Electronic-Structure Theory - Correlated Electron Materials

Time: Wednesday 18:15–20:30 Location: Poster A

O 82.1 Wed 18:15 Poster A

Implementation of the Strongly Constrained and Appropriately Normed Semilocal Density Functional (SCAN) with Self Interaction Correction (SIC) — •Lenz Fiedler, Jens Kortus, Torsten Hahn, and Sebastian Schwalbe — TU Freiberg, Institute for Theoretical Physics, Freiberg, Germany

Density Functional Theory (DFT) has become the most important computational method for the calculation of electronic structure. In order to calculate the exchange and correlation energy of a given system, there exists a wide variety of functionals. One of the recent developments in that area is the introduction of the SCAN functional [1]. Even such modern exchange-correlation functionals like SCAN are still subject to the self-interaction error [2]. The recently proposed Fermi-Löwdin orbital method for self-interaction correction (FLO-SIC)[3-4] seeks to correct this self-interaction error.

We therefore present the results of an implementation of the SCAN functional in the Naval Research Laboratory Molecular Orbital Library (NRLMOL). This implementation is used to verify the computational properties of the SCAN functional as well as to enable the combination of SCAN and FLO-SIC in order to further improve the results of DFT calculations.

[1] J. Sun, A. Ruzsinszky, J. Perdew, PRL, vol. 115, 036402 (2015)
[2] J. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)
[3] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[4] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)

O 82.2 Wed 18:15 Poster A

Fermi-Löwdin orbital self-interaction corrected DFT for molecules — •Jakob Kraus, Sebastian Schwalbe, Torsten Hahn, and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany

One of the more recent methods of addressing the self-interaction error (SIE) in density functional theory (DFT), namely the Fermi-Löwdin orbital self-interaction correction (FLO-SIC [1]), provides significant improvements in total energies, level ordering and ionization potentials [2]. Notably, the generated Fermi-Löwdin orbitals are suspected to hold actual chemical meaning. Furthermore, there is evidence implying that FLO-SIC results allow for an interpretation in terms of the Lewis formulae of common molecules. In this contribution, we deliver FLO-SIC structural formulae of neutral and charged diatomic molecules which, from a chemist's point of view, do not possess an adequate Lewis formula. Given these results, we propose a FLO-SIC-based bond order scheme.

[1] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)
[2] T. Hahn et al., JCP, vol. 143, 224104 (2015)

O 82.3 Wed 18:15 Poster A

Force balance equation and exchange-correlation potentials in time-dependent current density functional theory(tdCDFT) — •Mary-Leena Martine Tchenkoue Djouom, Markus Penz, Michael Ruggenthaler, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The Runge-Gross theorem as the conceptual basis of tdCDFT is based on a force balance equation from which the existence of a unique mapping between potentials (including a vector potential) on the one side and one-particle densities and currents on the other side is derived. Since tdCDFT is expected to solve important problems that persist in tdDFT (without regarding vector potentials and currents) the study of this force equation is of special interest. Here we use the force balance equation to derive approximate exchange-correlation potentials that obey basic conditions such as zero-force and zero-torque. Such approximations will be useful in the calculation of dynamical properties of many-particle systems.

O 82.4 Wed 18:15 Poster A

Reliable magnetic properties for spin-crossover complexes with Fermi-Löwdin orbital self-interaction corrected DFT ? — •Julia Richter, Sebastian Schwalbe, Jens Kortus, and Torsten Hahn — TU Freiberg, Institute for Theoretical Physics, Germany

Octahedral Fe^{2+} molecules are particularly interesting as they often exhibit a spin-crossover transition. The existing semilocal exchange-correlation functionals used in density functional theory (DFT) calculations are known to fail badly in predicting the energy differences between the various spin states of these molecules. We apply the recently developed Fermi-Löwdin orbital self-interaction correction (FLO-SIC) [1,2] to $[Fe(H_2O)_6]^{2+}$, $[Fe(NH_3)_6]^{2+}$, $[Fe(NCH)_6]^{2+}$ and $[Fe(CO)_6]^{2+}$ complexes and we benchmark against non-SIC corrected DFT and diffusion Monte Carlo results [3]. We expect, that the correct treatment of the exchange energy within the FLO-SIC method leads to improved description of spin states.
[1] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[2] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)
[3] Droghetti, A. et. al., J. Chem. Phys., vol. 137, 124303 (2012).

O 82.5 Wed 18:15 Poster A

Towards chemical accuracy of FLO-SIC — •Sebastian Schwalbe[1], Torsten Hahn[1], Simon Liebing[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany — [2]Central Michigan University, Department of Physics, USA

Fermi-Löwdin orbital self-interaction correction (FLO-SIC) [1,2,3] is applied to atoms and molecules as defined in the standard G2-1 test set. Within this systematic study calculated ionization potentials and binding energies are compared with experimental values. It will be shown that the FLO-SIC method provides significant improvements towards chemical accuracy by using the framework with the LSDA functional, but noteworthy worse performance in combination with the PBE-GGA or other GGA functionals.

[1] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)
[2] T. Hahn et al., JCP, vol. 143, 224104 (2015)
[3] T. Hahn et al., JCTC (2017)

O 82.6 Wed 18:15 Poster A

Improvements for FLO-SIC: Electron force field (eFF) and Frozen-Core Approximation — •Sebastian Schwalbe[1], Simon Liebing[1], Kai Trepte[2], Torsten Hahn[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany — [2]Central Michigan University, Department of Physics, USA

The Fermi-Löwdin orbital self-interaction correction (FLO-SIC) [1,2,3] is computational limited by the time needed for the optimization of reference positions in real space, namely the Fermi-Orbital-descriptors (FODs). Using the electron force field (eFF) for pre-optimization of these positions enables a significant speed-up of any FLO-SIC calculation. Further, the authors give a short review on other speed-up possibilities. In particular a so called Frozen-Core FLO-SIC method is discussed. Finally, a general speed-up methodology combining all the aforementioned techniques is proposed.

[1] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)
[2] T. Hahn et al., JCP, vol. 143, 224104 (2015)
[3] T. Hahn et al., JCTC (2017)

O 82.7 Wed 18:15 Poster A

Ab-initio structural relaxation of molecular crystals under pressure — •Eric Pierschel — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Germany

The structural relaxation of molecular crystals presents serious difficulties. In principle, forces acting on the atoms, calculated as energy gradients, allows for the search of the molecular configuration with the minimum possible energy. The drawback of this method is that the forces between atoms belonging to a single molecule are significantly stronger than the ones between atoms in different molecules. This makes the numerical determination of the orientation of molecules with respect to each other very difficult. To avoid this problem, we use a cluster algorithm which, first, detects individual molecules. Then, independent translations and rotations for each molecule are added to the list of the standard $3N$ degrees of freedom, corresponding to the N atoms in the unit cell. The structure optimization is performed in this overdetermined parameter space by using the BFGS-algorithm. Optionally, our procedure allows for performing the optimization of the molecular degrees of freedom only, by considering each molecule as a rigid rotator. We use this approach for relaxing molecular crystals, like the oligo-acens, under pressure. *Ab-initio* total energies are calculated using density-functional theory including van-der Waals interactions as implemented in the full-potential all-electron code `exciting`.

O 82.8 Wed 18:15 Poster A

FLO-SIC DFT applied to pseudopotentials — •Simon Liebing, Sebastian Schwalbe, Torsten Hahn, and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany

A method bases on Fermi-Löwdin orbitals to correct the self-interaction error within DFT (FLO-SIC) was developed by Pederson and co-workers. [1,2,3] The authors show how the FLO-SIC method can be used within the pseudopotential methodology. The calculation speedup and accuracy in comparison with all-electron calculations are discussed in detail. The FLO-SIC pseudopotential scheme leads to a similar improvement of the ionization potentials, eigenvalues and bond energies compared to the all-electron variant.

[1] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)
[2] T. Hahn et al., JCP, vol. 143, 224104 (2015)
[3] T. Hahn et al., JCTC (2017)

O 82.9 Wed 18:15 Poster A

Self-energy self-consistency within density functional theory + dynamical mean field theory — •Sumanta Bhandary[1] and Karsten Held[2] — [1]Centre de Physique Thèorique, Ecole Polytechnique, 91128 Palaiseau, France — [2]Institute of Solid State Physics, TU Wien, 1040 Wien, Austria

We study the effects of self-energy self-consistency within a framework combining density functional theory (DFT; Wien2k) and dynamical mean field theory (DMFT; w2dynamics) in a basis of maximally localized Wannier orbitals. In addition to the charge density correction in DFT+DMFT charge self-consistency [1], in this scheme, we re-write the DFT exchange correlation potential in a form of a local self-energy, obtained in DMFT. The method is applied to transition metal oxides, involving a so called $d+p$ calculations. The overestimated $d-p$ hybridization in DFT is greatly improved, correcting the relative energy positions of the d and the p orbitals. Importantly, in this methodology, the explicit form of the exchange correlation potential is known and hence the ambiguity of the troublesome 'double-counting' term in regular DFT+DMFT formalism is avoided.

[1] S. Bhandary, E. Assmann, M. Aichhorn, and K. Held, Phys. Rev. B **94**, 155131 (2016).

O 82.10 Wed 18:15 Poster A

Vacancy charged defects in two-dimensional GaN: An ab-initio study — •Rafael Gonzalez-Hernandez[1], William Lopez-Perez[1], Alvaro Gonzalez-Garcia[1], and Maria Guadalupe Moreno Armenta[2] — [1]Depament of Physics, Universidad del Norte, Barranquilla, Colombia — [2]Centro de Nanociencias y Nanotecnología-UNAM, Km 107 carretera Tijuana-Ensenada, Ensenada, México

In this work, we have studied the structural and electronic properties of vacancy charged defects in the graphene phase (honeycomb type) of gallium nitride (g-GaN) by using first-principles calculations within the framework of the Density Functional Theory [1]. It is found that the vacancies introduce defect levels in the band gap, and these generate a total magnetization in the g-GaN system. The formation energy with different charge states for the vacancies of gallium and nitrogen were calculated, obtaining higher energies than the GaN wurtzite phase (w-GaN). Furthermore, nitrogen vacancies were found to be more stable than gallium vacancies in a whole range of electronic chemical potential. Gallium and nitrogen vacancies produce a nonzero magnetic moment in g-GaN, making it a potential candidate for future spintronics applications. In addition, free-standing g-GaN has been overcome by Al Bolushi et al. [2] using a migration-enhanced growth (MMEG) method in which two- dimensional GaN layers are created beneath the graphene layer generated by the Si sublimation form SiC(0001) sample.

References [1] Giannozzi et al., J. Phys.:” Condens. Matter 21 (2009) 395502 [2] Z. Al Balushi et al, ”Two-dimensional gallium nitride realized via graphene

O 82.11 Wed 18:15 Poster A

Convergence of Kohn-Sham construction in lattice tdDFT — •Benedikt Mehmel, Michael Ruggenthaler, Markus Penz, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg

In this master project we use the simple model of a two-site lattice system with two interacting particles to study the mathematical properties of the Kohn-Sham system in time-dependent density function theory. The necessary functional analytic tools include Fréchet differentiability and they are employed to show convergence of the self-consistent Kohn-Sham construction as a fixed point scheme. Such tools are also used to study the possibilty of a Runge-Gross theorem via the inverse function theorem applied to the potential-density map. As a side product exact conditions on possible approximations to the exchange-correlation potential in the scope of this simple model are established.

O 82.12 Wed 18:15 Poster A

Density Response to a Phonon Perturbation from DFPT Using the All-Electron FLAPW Method — •Christian-Roman Gerhorst, Markus Betzinger, Gustav Bihlmayer, Daniel Aaron Klüppelberg, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

A significant milestone in the calculation of phonon dispersions within Density Functional Perturbation Theory (DFPT) is the self-consistent solution of the Sternheimer equation. The resulting expansion coefficients of the response of the wavefunctions describe the linear variation of the density induced by a phonon perturbation. Using the all-electron Full-potential Linearized Augmented Plane-Wave (FLAPW) method, as implemented in the FLEUR code, enables an accurate treatment of complex materials without approximations to the 1/r potential or to the core electrons, but at the expense of additional conceptual challenges due to atom-positioned basis functions. In this contribution, we resolve computational challenges and show results of the self-consistently iterated Sternheimer equation reporting especially on the first variation of the density due to a phonon perturbation. In addition, we briefly shed light on the second-order quantities required for the dynamical matrix and focus on how the choice of the FLAPW method influences the shape of their equations.

O 82.13 Wed 18:15 Poster A

Calculating temperature-dependent resistivities in the KKR formalism: Implementation and application to simple metals — Carsten Eberhard Mahr, •Michael Czerner, and Christian Heiliger — Justus-Liebig-University, Giessen, Germany

Electron-phonon coupling is one of the main incoherent scattering mechanisms in a wide variety of crystalline material systems at room temperature and above. Therefore, it is necessary to incorporate those effects in any realistic calculations of electronic transport properties. To do so, we have recently reported [Phys. Rev. B 96, 165121 (2017)] an extension to our density functional theory (DFT) based Korringa-Kohn-Rostocker (KKR) Green's function formalism code.

By approximating the Fröhlich-type interaction by a suitably wave-vector-averaged energy-dependent self-energy Σ_{eph} we are able to compute the dressed propagator $G = G_{\mathrm{ref}} + G_{\mathrm{ref}} \cdot \big(\Delta V + \Sigma_{\mathrm{eph}}\big) \cdot G$ by solving Dyson's equation, where G_{ref} is the Green's function of an arbitrary (though typically repulsive) reference system. The averaged self-energy is extracted from first principles electron linewidth calculations employing Quantum ESPRESSO and EPW.

We demonstrate the physical validity of the beforementioned calculational scheme for non-equilibrium properties by comparing evaluated temperature-dependent resistivities of copper and aluminum to experimental data. Further, technical details of the implementation in the KKR basis set are presented.

O 82.14 Wed 18:15 Poster A

Developing Density Functional Based Tight-Binding Methods within a Self-Consistent Field Density Functional Theory Framework — •Frederick Stein, Jens Kunstmann, and Gotthard Seifert — TU Dresden, Germany

The Density-Functional Tight-Binding (DFTB) method is an approximate density functional theory scheme that is routinely used in computer simulations with large system sizes or long simulation times. The method traditionally exists in a non-selfconsistent (DFTB0) and a charge-selfconsistent (SCC-DFTB) flavor. Here we develop a self-consistent field DFTB (SCF-DFTB) scheme that is very general and directly allows improvements of traditional DFTB methods. We demonstrate how the SCC-DFTB formalism can be derived from SCF-DFTB without the use of a second-order expansion of the total energy. This leads to a new interpretation of SCC-DFTB and the involved Hubbard parameter in terms of a flexible basis set. Furthermore we use small molecules to study SCF-DFTB variants with spherical and non-spherical corrections of the DFTB0 Hamiltonian. Our results indicate that the success of DFTB is based on multiple, well-balanced approximations. Attempts to only correct individual approximations are not leading to better results.

O 82.15 Wed 18:15 Poster A

Considerations About the Gauge Factor in TDDFT-Ehrenfest MD with Non-Local Pseudopotentials — •Lukas Deuchler and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, CAU Kiel

It is well known that non-local pseudopotentials (PPs) require a gauge factor when a vector potential is introduced into the Kohn-Sham equations [1]. In PP-based TDDFT-Ehrenfest molecular dynamics simulations, the motion of the ions leads to a similar issue [2,3]. In case of norm-conserving PPs, which are applied in the fully separable Kleinman-Bylander form, Avendaño-Franco has stated in his thesis [4] that the non-local PP has to be multiplied by a phase factor with a phase proportional to the ion velocity to derive the dynamic ground state for TDDFT-MD. Here we argue that Galilei invariance of the TDDFT equation of motion requires this gauge factor to be applied to the non-local PP during the time propagation of the Kohn-Sham states. Quantitatively, the effect of omitting the gauge factor during propagation (while still correctly including the initial boost of the Kohn Sham states) appears to be small in case of the semilocal Troullier-Martins PPs we have tested, consistent with [4]. The TDDFT-MD calculations have been carried out with the code Octopus [5].

[1] Bertsch et al., Phys. Rev. B 62, 7998 (2000).

[2] Qian et al., Phys. Rev. B 73, 035408 (2006).

[3] Ojanperä et al., J. Chem. Phys. 136, 144103 (2012).

[4] Avendaño-Franco, PhD Thesis, UC Louvain (2013).

[5] Andrade et al., Phys. Chem. Chem. Phys. 17, 31371 (2015).

O 83: Poster Focus Session: Structural Dynamics in Nanoscale Materials, Probed by Ultrafast Electron Pulses

Time: Wednesday 18:15–20:30 Location: Poster A

O 83.1 Wed 18:15 Poster A

Energy relaxation and dissipation in laser-excited thin film heterostructures — •K. Sokolowski-Tinten[1], R. Li[2], A. H. Reid[2], X. Shen[2], Q. Zheng[2], T. Chase[2], M. Milnikel[1], R. Coffee[2], J. Corbett[2], H. Dürr[2], N. Hartmann[2], C. Hast[2], R. Hettel[2], M. Horn-von Hoegen[1], D. Janoschka[1], M. Jermann[1], M. Ligges[1], I. Makasyuk[2], M. Mo[2], F. Quirin[1], B. Rethfeld[3], S. Salamon[1], A. Terwey[1], T. Veccione[2], U. von Hörsten[1], S. P. Weathersby[2], H. Wende[1], C. Witt[1], and X. Wang[2] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany. — [2]SLAC Nat. Acc. Lab., Menlo Park, USA. — [3]Dep. of Physics and OPTIMAS Research Center, TU Kaiserslautern, Germany

We use time-resolved MeV transmission electron diffraction experiments to study the incoherent structural response of nanoscale materials after fs laser excitation. Experiments were carried out using the MeV Ultrafast Electron Diffraction (UED) facility recently established at SLAC [1]. UED@SLAC provides ultrashort <300fs electron pulses at relativistic energies (3-5 MeV), which we have used for precise measurements of the transient Debye-Waller-effect in different metal-insulator and metal-metal-heterostructures, highlighting the importance of interface [2] and transport effects.

[1] S. P. Weathersby et al., Rev. Sci. Instrum. 86, 073702 (2015).

[2] K. Sokolowski-Tinten et al., New J. Phys. 17, 113047 (2015); Struct. Dyn. 4, 054501 (2017).

O 83.2 Wed 18:15 Poster A

Ultrafast electron diffraction with RF-compressed electron pulses — •Marius Milnikel[1], Patrick Lapsien[1], Martin Otto[2], Laurent P. René de Cotret[2], Nico Rothenbach[1], Soma Salamon[1], Alexandra Terwey[1], Ping Zhou[1], Bradley J. Siwick[2], Heiko Wende[1], and Klaus Sokolowski-Tinten[1] — [1]University of Duisburg-Essen and Centre for Nanointegration Duisburg-Essen, Faculty of Physics, Lotharstraße 1, 47057 Duisburg, Germany — [2]Department of Chemistry, McGill University, 801 Sherbrooke St., Montreal, Quebec, Canada

One of the major challenges in ultrafast electron diffraction (UED) is the electron pulse broadening induced by space-charge effects at high bunch charge. It has been demonstrated that the linear chirp introduced by this effect allows re-compression of the electron pulses to a pulse duration of about 100 fs by a time-dependent electrical field using a radio-frequency cavity at bunch charges of up to 10^6 electrons [1,2]. Here we report about our current efforts to set up such a RF-compressed electron source based on the concept introduced in [1], which has been recently commercialized [3]. Additionally we will present results of time-resolved diffraction experiments on metal-insulator heterostructures performed at the RF-compressed short pulse electron source at McGill University [2].

[1] van Oudheusden et al, Phys. Rev. Lett. 105, 264801 (2010).

[2] Chatelain et al., Appl. Phys. Lett. 101, 081901 (2012).

[3] AccTec BV: "A poor man's X-FEL" (www.acctec.nl/acctec.nl/index.php/products/).

O 83.3 Wed 18:15 Poster A

Picosecond acoustic waves in laser-excited metal-semiconductor heterostructures studied by ultrafast X-ray diffraction — •Fabian Brinks[1], Mohammadmahdi Afshari[1], Philipp Krumey[1], Andrey Akimov[2], Dmitri Yakovlev[3], Manfred Bayer[3], and Klaus Sokolowski-Tinten[1] — [1]Faculty of Physics and Centre for Nanointegration Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg — [2]School of Physics and Astronomy, University of Nottingham, NG7 2RD, UK — [3]Faculty of Physics, Technical University Dortmund, 44221 Dortmund, Germany

Absorption of ultrashort optical pulses in solids leads to a quasi-instantaneous increase of stress/pressure which is subsequently released by acoustic strain waves traveling through the sample. We investigate the excitation and transient evolution of such coherent acoustic phonons in metal-semiconductor heterostructures composed of thin metal films (Ti, Cr, Al, Al, Pt, Au, Pd) deposited on 100-oriented GaAs substrates by time-resolved X-ray diffraction using ultrashort X-ray pulses at 4.5 keV from a fs laser-plasma X-ray source. By probing the GaAs (400) Bragg reflection in an optical pump - X-ray probe scheme and comparing our experimental data to dynamical diffraction calculations, we aim to develop a quantitative material-dependent understanding of the transient stress/strain evolution upon ultrafast laser excitation.

O 83.4 Wed 18:15 Poster A

Towards observing dynamics in molecular overlayers using Ultrafast Low Energy Electron Diffraction (ULEED) — •Bareld Wit, Erica Warth Pérez Arias, Theo Diekmann, Gerrit Horstmann, Simon Vogelgesang, Gero Storeck, and Claus Ropers — 4th Physical Institute, University of Göttingen, 37077 Göttingen, Germany

Very recently, we reported the successful implementation of ULEED in backscattering mode. This yielded new insights into the model system of charge density wave dynamics in 1T-TaS2 [1,2]. One of the next challenges is to expand the scope of ULEED to dedicated surface systems for which the structural dynamics cannot be accessed by other time resolved techniques. In this contribution, the progress towards resolving ultrafast dynamics in (sub-)monolayer molecular overlayers on solid substrates will be presented.

As a model system, we have chosen 1,2-bis(4-pyridyl)ethylene (bpe) on graphite. It has been shown that bpe forms ordered islands at sub-monolayer coverages that can reversibly melt at 414K [3]. We can observe this 'order-disorder' transition with LEED. Moreover, since the transition is reversible, it is in principle suited for pump-probe experiments yielding ultrafast structural dynamics.

[1] S. Vogelgesang et al., Nature Phys. doi:10.1038/nphys4309 (2017)

[2] G. Storeck et al., Struct. Dyn. 4, 044024 (2017)

[3] A. Y. Brewer et al., Mol. Phys. 111, 73 (2013)

O 83.5 Wed 18:15 Poster A

Nonequilibrium dynamics of laser excited SiC: Description of Laser excited SiC with the help of classical physics — •Malwin Xibraku, Bernd Bauerhenne, Sergej Krylow, and Martin E. Garcia — University of Kassel, Theoretical Physics, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Silicon carbide (SiC) nanocrystals are of great interest in medicine, because of their pleasant properties, such as biocompability, high chemical and thermal stability. These nanocrystals can be very well generated using ultrashort laser pulses. Density Functional theory (DFT) has proven to be a appropriate tool to describe the influence of ultrashort laser pulses on solids due to the accurate quantum mechanical treatment of electrons. Due to the fact that 48 million particles are already contained in a cube SiC of side length 100 nm, such a system cannot be computed with DFT. Therefore, the aim of this work is to describe the forces between the atoms in the SiC cube by an effective potential in the context of classical physics. The classical potential should include the effect of the quantum properties of electrons as accurately as possible. Recently, we found such a potential for silicon (Si) and carbon (C). Therefore, the main goal of this work is to generalize the shape of those potentials to solids consisting of two types of atoms. We propose a general shape of a potential for laser excited binary solids and obtain the coefficients by fitting to data obtained from ab initio simulations on small supercells of SiC. We discuss the quality of the obtained potential by comparing MD simulations performed both with the potential and ab-initio.

O 83.6 Wed 18:15 Poster A

Ultrafast electron dynamics in free space controlled by femtosecond laser pulses — •Norbert Schönenberger, Martin Kozák, Joshua McNeur, Peyman Yousefi, and Peter Hommelhoff — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Pulsed electron beams are a unique probe for ultrafast studies of condensed matter systems, since they allow for both high spatial and temporal resolution. Light in the visible or near-infrared is an ideal candidate for controlling these electrons on single-femtosecond or even attosecond timescales. This can be achieved using electromagnetic near-fields created at dielectric structures, so called dielectric laser accelerators (DLAs) [1]. In recent years, these devices have gained attention with the goal to build fully photonic particle accelerators. We report on new structures allowing better transverse control of the electron beam, leading to a more homogeneous interaction and providing a higher acceleration gradient. Furthermore, we present a technique for inelastic scattering of electron at a light wave in free space [2]. Two laser pulses are used to form an optical travelling wave that interacts with the electrons via ponderomotive scattering, provided that the parameters are chosen for the proper phase-matching. Both methods show promise for creating high-energy attosecond probes for the future ultrafast diffraction and microscopy research.

[1] Kozak M., McNeur J., et.al: Nat. Comms 8 (2017), DOI: 10.1038/ncomms14342 [2] Kozák, M., Eckstein, T., Schönenberger, N. & Hommelhoff, P., Nat. Phys. (2017), DOI: 10.1038/NPHYS4282.

O 83.7 Wed 18:15 Poster A

Ultrashort electron pulses in the space charge regime — •Nora Bach[1], Till Domröse[1], Armin Feist[1], Claus Ropers[1], and Sascha Schäfer[1,2] — [1]4th Physical Institute, Georg-August-University, Göttingen, Germany — [2]Institute of Physics, University of Oldenburg, Germany

Ultrafast transmission electron microscopy (UTEM) has become a powerful tool to investigate processes on the nanoscale with femtosecond temporal resolution [1]. The Göttingen UTEM is based on the modification of a commercial Schottky field emission TEM for which single-photon photoemission from a tip-shaped ZrO/W(100) emitter is employed. Spatial resolution down to the sub-nanometer regime and a spectral bandwidth of 0.6 eV is provided [2].

Here, we investigate the influence of the photoemitted electron density on the resulting transverse and longitudinal beam properties. For constant laser pulse duration, both emittance and energy width scale linearly with pulse charge. For increasing duration, however, both quantities decrease. Simulated results are in good agreement with the experimental data. The demonstrated high beam quality of the source and its tunability 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] A. Feist et al., Ultramicroscopy 176 (2016)

O 83.8 Wed 18:15 Poster A

Ultrafast transmission electron microscopy using laser-triggered field emitters — •Thomas Danz[1], Armin Feist[1], Nara Rubiano da Silva[1], Marcel Möller[1], Nora Bach[1], Sascha Schäfer[1,2], and Claus Ropers[1] — [1]IV. Physical Institute – Solids and Nanostructures, University of Göttingen, Germany — [2]Institute of Physics, University of Oldenburg, Germany

Ultrafast transmission electron microscopy (UTEM) is a promising approach to investigate structural, electronic, and magnetic dynamics with nanometer spatial and femtosecond temporal resolution in a laser pump/electron probe scheme using the versatile imaging, diffraction, and spectroscopy capabilities of such an instrument [1–3].

The pulsed electron source of the Göttingen UTEM project employs linear photoemission from a nanoscopic Schottky emitter, delivering highly coherent electron pulses with down to 200 fs pulse duration, 0.6 eV energy width, and sub-1 nm focused beam diameter [4]. Here, we discuss the present status of the Göttingen UTEM along with selected applications in ultrafast electron imaging and diffraction.

[1] A. H. Zewail, Science **328**, 187 (2010).

[2] A. Feist *et al.*, arXiv:1709.02805, accepted for publication in *Structural Dynamics*.

[3] N. Rubiano da Silva *et al.*, arXiv:1710.03307.

[4] A. Feist *et al.*, Ultramicroscopy **176**, 63 (2017).

O 83.9 Wed 18:15 Poster A

Ultrafast Microscopy of Charge Carrier Motion in Nanoscale Systems — •Faruk Krecinic[1], Melanie Müller[1], Jannik Malter[1], Alexander Paarmann[1], Vasily Kravtsov[2], Markus Raschke[2], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]University of Colorado, Boulder, USA

The ultrafast motion of charge carriers at the nanoscale plays a crucial role in our understanding of optoelectronic systems. We recently developed femtosecond point projection microscopy (fs-PPM) as a new technique for visualizing ultrafast charge carrier motion with nanometer resolution [1]. Due to the use of low-energy electrons, the fs-PPM image is highly sensitive to local electric fields. Here we present our recent experiments visualizing the photoionization of silver nanowires excited with intense laser fields. The dynamics of the photoelectrons and the concomitant positive charging of the nanowires is shown to happen on a time scale as short as 40 fs. The field sensitivity of this technique can be further enhanced, down to the level of a single elementary charge, by taking advantage of the phase information of the imaging electron wavepacket, i.e. by performing electron holography. Our recent progress toward the development of femtosecond low-energy electron holography will also be reported. [1] M. Müller et al., Nature Comm. 5, 5292 (2014).

O 83.10 Wed 18:15 Poster A

Harmonicity and anharmonicity of phonon and surface phonon-polariton in high symmetry directions in wurtzite AlN — •Hrag Karakachian[1,2] and Michel Kazan[1] — [1]Department of Physics, American University of Beirut, P.O. Box 11-0236, Riad El-Solh, Beirut 1107-2020, Lebanon — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

We report on the potential of self-nucleated AlN single crystal as a tunable near-field infrared source. The grown crystal exhibits natural AlN growth characteristics with several well-developed facets of different orientations. The characteristics of surface-phonon-polariton (SPhP) modes on the developed crystal facets have been investigated. Reflectivity spectra were recorded from five facets of different orientations. The measured spectra were analyzed by a model taking into account the dependence of harmonicity and anharmonicity of the excited zone center optical phonons on the surface orientation. Consequently, the dielectric properties that determine the condition of existence, dispersion relations, and lifetimes of the SPhP modes were accurately retrieved. The dielectric functions were determined as a function of the angle of incidence and used to compute the characteristics of the SPhP modes on each of the measured facets. We found that facets of different orientations exhibit SPhP modes of different frequencies and lifetimes, which makes the investigated self-nucleated crystal potential candidates for tunable near-field infrared sources.

O 84: Poster Focus Session: Structure and Chemistry of Metal-Oxide Surfaces

Time: Wednesday 18:15–20:30 Location: Poster A

O 84.1 Wed 18:15 Poster A

Adsorption of O_2 on Rutile (110) surface studied by Atomically-resolved AFM/STM — •Igor Sokolovic, Martin Calkovsky, Michael Schmid, Ulrike Diebold, and Martin Setvin — TU Wien, Institute of Applied Physics, Wiedner Hauptstr. 8-10/134, 1040 Vienna, Austria

The Rutile TiO_2 (110) surface is a well-studied surface, which makes it an excellent model system for testing new methods. O_2 adsorption on this surface has been studied by many techniques [1] - [4], yet there are still controversies even about the basic O_2 adsorption configurations. This contribution will show that a combined non-contact qPlus atomic force microscopy (AFM) and scanning tunneling microscopy (STM) setup provides a powerful tool for direct imaging and manipulating the adsorbed molecules. The AFM allows for completely non-intrusive measurements, showing three distinct molecularly adsorbed O_2 species. Applying sample bias results in dissociation, desorption or configuration change of the adsorbed molecules. The role of sample and dosing temperature is discussed. The adsorbates are also investigated with Kelvin probe spectroscopy and force spectroscopy. The effect of electrons and holes induced by ultraviolet light irradiation is investigated for the various adsorbed species.

References: [1] Diebold, U. Surface science reports 48.5 (2003): 53-229. [2] Du, Y., et al. The Journal of Physical Chemistry C 112.7 (2008): 2649-2653. [3] Petrik, N.G., et al. The Journal of Physical Chemistry Letters 1.12 (2010): 1758-1762. [4] Henderson, M.A., et al.

The Journal of Physical Chemistry B 103.25 (1999): 5328-5337.

O 84.2 Wed 18:15 Poster A

Roughening prevention in reactive ion beam figuring of aluminium mirror surfaces — •Jens Bauer, Melanie Ulitschka, Frank Frost, and Thomas Arnold — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Mirror optics for short-wavelength imaging applications demand superior optical surface properties, i.e. a high figure accuracy down to the atomic level as well as a low surface micro-roughness below 1 nm rms. Up to now it is not possible to meet those requirements by direct machining of optical Al surfaces made from technical alloy materials as AL6061 or AL905. Conventional machining technologies fail, since the surface roughness increases drastically as a result of structural, crystallographic and chemical matrix irregularities. Recently has been shown, that ultra-precision machining by reactive ion beams can be a promising approach for surface figuring without considerable increase of the surface roughness. Based on process investigations by WLI, AFM, and TOF-SIMS and supplemented by Monte Carlo simulations a phenomenological model is suggested. In particular, the usage of O_2 or N_2 containing process gas induces the formation of a homogeneous and temporally stable surface oxide or nidride layer, respectively. This layer results from a quasi-stationary equilibrium between ion implantation and sputter erosion due to the impact of the energetic reactive ions. The surface layer acts as an etching front moderating the inhomogeneous structural conditions of the aluminium bulk material. As a result, by use of reactive ion beams the surface roughness can now be preserved in its initial state during ultra-precision figure correction.

O 84.3 Wed 18:15 Poster A

Electronic and reactive properties of alloyed Au_xPd_y nanoparticles on TiO_2 supports — •Xiaojuan Yu, Alexei Nefedov, Christof Wöll, and Yuemin Wang — Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany.

PdAu bimetallic catalysts have been shown to display enhanced catalytic activities and selectivities compared with their monometallic counterparts in a variety of reactions. However, the nature of the improved catalytic performance of alloyed PdAu nanoparticles (NPs) is still under debate. Here we present the results of a thorough study on various monometallic and bimetallic Au_xPd_y-TiO_2 nanoparticles (x:y = 1:0, 7:3, 1:1, 3:7, 0:1) using primarily ultrahigh vacuum IR spectroscopy (UHV-FTIRS) in conjunction with photoelectron spectroscopy (XPS). The different surface sites of monometallic and bimetallic Au-Pd NPs supported on TiO_2 powders were identified by UHV-FTIRS using CO as a probe molecule. For monometallic Au and Pd NPs, the positively charged $Au^{\delta+}$ and Pd^{2+} were detected as majority of species, while for bimetallic AuPd NPs, Au^0, atop Pd^0 and bridge Pd^0become the dominating species. The strong electronic interaction between Au and Pd in the alloyed AuPd NPs was demonstrated based on the XPS results and the frequency shift of the corresponding CO bands. The catalysis experiments revealed that the Au_3Pd_7-TiO_2 sample exhibits the highest activity for CO oxidation. This was attributed to the activation of molecular oxygen at the enriched Pd species.

O 84.4 Wed 18:15 Poster A

IRRAS studies of CO adsorption on well-defined iron oxide surfaces — •Ludger Schöttner, Alexei Nefedov, Chengwu Yang, Stefan Heissler, Yuemin Wang, and Christof Wöll — Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen

The interaction between CO and iron oxide (Fe_2O_3, hematite, and Fe_3O_4, magnetite) surfaces is of great interest because of its applications in heterogeneous catalysis and industrial processes such as carbothermic iron ore reduction. In addition, CO is the simplest heteronuclear diatomic molecule and is widely used in infrared spectroscopy (IR) to probe the local structure of catalyst surfaces. In this work the adsorption of CO on various iron oxide monocrystalline surfaces was studied using polarization-dependent IR reflection absorption spectroscopy (IRRAS). Based on the IRRAS results, it was established that the stoichiometric surface of $Fe_2O_3(0001)$ is terminated with Fe^{3+}, as observed for the $Fe_3O_4(001)$ surface. On the $Fe_3O_4(111)$ surface two vibrational CO bands were detected which correspond to Fe^{3+} and Fe^{2+} species, respectively. It was found that after reduction the hematite (0001) surface is converted to the more stable magnetite (111) structure. Moreover, the magnetite (111) facets were identified as a primary topology on the reconstructed $Fe_3O_4(110)$ surface.

O 84.5 Wed 18:15 Poster A

Chemical Reactivity of Amorphous Oxide Surfaces — •Hannah Schlott and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Theoretical studies on the chemical reactivity of surfaces have been performed almost exclusively for crystalline model surface structures. When it comes to oxides, however, surfaces are typically amorphous and are covered by residuals from the environment, in particular OH groups from contact with water or protective ligand shells in the case of nanoparticles. Using Car-Parrinello Molecular Dynamics (CPMD) we first prepared amorphous ZnO and TiO_2 surface structures and subsequently studied their chemical reactivity by exposing them to a variety of small molecules, in particular, water and small organic molecules. The amorphous structures were generated by melt-quench simulations starting from randomly positioned metal and oxygen atoms in a supercell. The volume of the supercell was adjusted such that the experimental density of ZnO and TiO_2 was reproduced. A special new technique was developed that allows to create amorphous surface structures in a direct way without the need to cleave amorphous bulk configurations. First results for the interaction of water and acetic acid with the amorphous surfaces will be shown and will be compared to their behavior on the crystalline counterparts.

O 84.6 Wed 18:15 Poster A

Adsorption of catechol-derivatives on ZnO surfaces — •Tobias Müller and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

The physical and chemical properties of ZnO nanoparticles can be tuned by suitable ligand shells. Catechols are promising linker units since they are able to displace acetate ions from the ZnO surfaces which have remained from the wet-chemical ZnO nanoparticle synthesis. To obtain further insights into the competition of the binding strength of different linker groups on ZnO we have studied the adsorption structure and energy of three catechol derivatives (phenyl rings with one, two or three OH groups) and of acetate using density functional theory (DFT). The crystalline, nonpolar $ZnO(10\bar{1}0)$ wurtzite termination and three different amorphous model ZnO surface structures were considered. Particular attention was given to the investigation of different adsorption sites. The amorphous surfaces show a few highly reactive surface sites, but most other sites are less reactive than the crystalline surface. For the crystalline termination also the effect of higher surface coverages was investigated by increasing the surface coverage to 0.5, 0.75 and 1 monolayer. A thermodynamic analysis, which includes experimental temperature and pressure conditions via a chemical potential, shows that the saturation coverage is about 0.5 monolayers for all three catechol derivatives. Finally, the results are compared to experimental findings.

O 84.7 Wed 18:15 Poster A

Measuring the work function of ultrathin FeO(111) films on Ag(111) using STM — •Ying Wang, Visnja Babacic, and Mikolaj Lewandowski — NanoBioMedical Centre, Adam Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland

Ultrathin films constitute a new class of 2D materials which, due to finite size effects, exhibit unique physical and chemical properties not observed for the corresponding bulk materials. It was experimentally and theoretically shown that ultrathin FeO(111) films grown on Pt(111) exhibit superior catalytic activity in the CO oxidation reaction as compared to clean Pt(111) [J. Catal 266 (2009) 359; Angew. Chem. Int. Ed. 49 (2010) 4418]. This enhanced activity was found to be related, among other factors, to the work function of the FeO(111)/Pt(111) system. We used scanning tunneling microscopy (STM) operating in dI/dz spectroscopy mode to measure the work function of ultrathin FeO(111) films grown on Ag(111). The results are compared to those obtained for FeO(111) on Pt(111).

Acknowledgment: The "Multifunctional ultrathin Fe(x)O(y), Fe(x)S(y) and Fe(x)N(y) films with unique electronic, catalytic and magnetic properties" project is carried out within the First TEAM programme of the Foundation for Polish Science (project number First TEAM/2016-2/14) co-financed by the European Union under the European Regional Development Fund.

O 84.8 Wed 18:15 Poster A

FeO(111) islands on Ru(0001): A potential catalyst for

the CO oxidation reaction — •Natalia Michalak[1,2], Zygmunt Milosz[1], Stefan Jurga[1], and Mikolaj Lewandowski[1] — [1]NanoBioMedical Centre, Adam Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland — [2]Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznan, Poland

Oxide films epitaxially grown on metal single crystal surfaces are widely used as model catalysts that allow deeper understanding of processes that occur on the surfaces of bulk oxide catalysts. We studied ultrathin FeO(111) islands epitaxially grown on Ru(0001) by room temperature iron deposition and post-oxidation in molecular oxygen. Such preparation leads to the formation of well-dispersed and well-ordered FeO(111) islands the size of which can be tuned by additional UHV annealing. Scanning tunneling microscopy (STM) operating in dI/dV mapping mode revealed the presence of potentially catalytically-active coordinatively unsaturated ferrous sites (CUFs) at the perimeter of the FeO islands and within the islands. The results indicate that FeO(111)/Ru(0001) can be a promising catalytic system for the CO oxidation reaction. Acknowledgement: This work was financially supported by the National Science Centre of Poland (PRELUDIUM project No. 2016/21/N/ST4/00302).

O 84.9 Wed 18:15 Poster A

Ordered and disordered surface vacancies on a ceria film surface — •Reinhard Olbrich[1], Gustavo E. Murgida[2,3], Valeria Ferrari[2,3], Clemens Barth[4], Ana M. Llois[2,3], Michael Reichling[1], and M. Veronica Ganduglia-Pirovano[5] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany — [2]Departamento de Física de la Materia Condensada, GIyA, CAC-CNEA, 1650 San Martín, Buenos Aires, Argentina — [3]Consejo Nacional de Investigaciones Científicas y Técnicas - CONICET, C1033AAJ, Buenos Aires, Argentina — [4]Aix-Marseille University, CNRS, CINaM UMR 7325, 13288 Marseille, France — [5]Instituto de Catálisis y Petroleoquímica, Consejo Superior de Investigaciones Científicas- CSIC, 28049 Madrid, Spain

Obtaining information about the defect structure of cerium oxide surfaces is of paramount importance in catalytic applications relying on the high oxygen storage capacity (OSC) of ceria.

We reveal surface vacancies on a 180 nm thick ceria film that arise from annealing in an ultra-high vacuum (UHV) environment at various temperatures up to 1100K by direct imaging with a non-contact atomic force microscope (NC-AFM). The oxygen vacancies can be separated in regularly arranged vacancies in form of surface reconstructions representing reduction stages ranging from CeO_2 to Ce_2O_3 and in vacancies appearing at disordered surface positions. We found that the disordered surface vacancies rearrange to some extend over time while the ordered vacancies are stable.

O 85: Poster: Tribology and Misc.

Time: Wednesday 18:15–20:30 Location: Poster A

O 85.1 Wed 18:15 Poster A

Frictional Behaviour of Colloidal Spheres Sliding on a Micron-Scale Periodic Substrate — •Alper Özoğul and Enrico Gnecco — Otto Schott Institute of Materials Research (OSIM), Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena, Germany

The Prandtl-Tomlinson model is widely used to explain the stick-slip nature of nanoscale friction on a crystal surface. Hence, the model is commonly associated with atomic-scale interactions, even though it can be in principle applied to any periodic 'tip-surface' interaction. To study the applicability of the PT model in micron scale, friction force between colloidal spheres of different materials (PMMA, SiO2, Borosilicate glass with Ø ~10 μm) attached to an AFM cantilever and a SiO2 grating consisting of 1.5 μm high slopes with a periodici-ty of 3 μm, is measured. The lateral deflection signals, which corre-spond to the friction force experienced by the spheres, are gathered in a variety of scan conditions (normal force set point, scan speed, sample orientation). As a result, friction force was found to vary up to an order of magnitude between different materials. The stick-slip behaviour characteristic of the PT model was clearly observed only with the PMMA spheres, whereas the friction is largely dominated by the sphere roughness and the surface topography with the other materials. Interestingly, we also observed that in all cases the friction is considerably reduced by contact oscillations superimposed to the scan motion, similarly to atomic-scale friction on crystal surfaces.

O 85.2 Wed 18:15 Poster A

Sonolubrication in Amorphous and Crystalline Materials — •Victor Pfahl[1], Chengfu Ma[2,1], Walter Arnold[3,1], and Konrad Samwer[1] — [1]I. Physikalisches Institut, Universität Göttingen — [2]Department of Precision Machinery and Precision Instrumentation, University of Science and Technology of China — [3]Department of Materials and Materials Technology, Saarland University

We studied sonolubricity, a phenomenon reducing friction between two sliding surfaces by ultrasound. Friction force measurements were performed in an atomic force microscope (AFM) when the tip-surface contact was excited to out-of-plane oscillations oscillations by a transducer or the built-in piezoelectric element in the cantilever holder.

Experiments were carried out near or at the first cantilever contact-resonance. We studied friction on crystalline and amorphous $Pd_{77.5}Cu_6Si_{16.5}$ ribbons, on a silicon wafer at room temperature, and on a $La_{0.6}Sr_{0.4}MnO_3$ thin film at different temperatures. Measurements were carried out varying the cantilever amplitude, the ultrasonic frequency, and the normal static load.

All experimental results display a universal behavior, which can be explained by the non-linearity of the force-distance curve between sample and tip due to the local interaction potential. An analytic function is found, which describes the reduction of friction as a function of the cantilever amplitude.

We would like to thank the DFG for funding CRC 1073 Project A1. Chengfu Ma gratefully acknowledges the China Scholarship Council for support.

O 85.3 Wed 18:15 Poster A

Indication of worn WC/C surface locations of a dry-running twin-screw rotor by the oxygen incorporation in tungsten-related Raman modes — •Henning Moldenhauer[1], Jörg Debus[1], Janina J. Schindler[1], Philipp Waldkirch[1], Sebastian Goeke[2], Andreas Brümmer[3], Dirk Biermann[2], and Manfred Bayer[1] — [1]Experimental Physics 2, TU Dortmund University, 44227 Dortmund, Germany — [2]Institute of Machining Technology, TU Dortmund University, 44227 Dortmund, Germany — [3]Chair of Fluidics, TU Dortmund University, 44227 Dortmund, Germany

Enhancing the lifetime of mechanical parts in industrial processes is a major goal. The key to enhancement is a tribological layer of several tens of namometer thickness that forms at the surface of the mechanical part. These surface changes during wearing have to be understood. This is done by identifying the composition of the tribological layer and determining its spatial distribution by using confocal Raman microscopy. Using this technique we study a tungsten-carbide/carbon (WC/C) surface of a dry-running twin-screw rotor, where worn and untouched locations are compared. Only at worn locations we observe tungsten-oxide Raman modes. Furthermore, several Raman lines are changed significantly in frequency and width, indicating mechanical distortion that occured during the wearing process. Specifically the Raman line at 680 cm^{-1} is enhanced, which corresponds to an incipient oxidation of the WC stretching mode. Given these findings, our results may be exploited to characterize the degree of wear of coated surfaces and to identify signatures of a tribological layer.

O 85.4 Wed 18:15 Poster A

Strahlen aus dem Zentrum von Lampen oder Sternen — •Theresa Ebner[1] und Lena Winterhalter[2] — [1]Ignaz-Günther-Gymnasium Rosenheim — [2]Ignaz-Günther-Gymnasium Rosenheim

Macht man bei Dunkelheit ein Foto von Sternen oder Lampen, sieht man aus dem Zentrum der Lampe oder des Sternes Strahlen kommen. Wodurch dieses Phänomen entsteht, welcher Zusammenhang zwischen Strahlenanzahl und Kamera besteht und warum wir diese Strahlen manchmal auch nur mit dem bloßen Auge sehen kann, habe ich erforscht und versucht zu erklären.

O 85.5 Wed 18:15 Poster A

Writing information in a self-assembled template of tetraphenylmethane derivatives using a scanning tunneling microscope — •Timo Frauhammer[1], Marcin Lindner[2], Michal Valasek[2], Lukas Gerhard[2], Marcel Mayor[2,3], and Wulf Wulfhekel[1,2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [3]Department of Chemistry, University of Basel, Switzerland

A self-assembled template of tetraphenylmethane derivatives adsorbed on a Au(111) surface, that exhibits a periodic arrangement of acetyl groups sticking out of the molecular film, is presented. By using the tip of a STM, these acetyl groups can be removed in a spatially controlled way without significantly affecting the remaining molecular assembly. The chemically modified molecules can be distinguished from the non-modified ones such that information can be engraved in the molecular film. The mesh size of this pattern can be tailored by varying the length of the molecular spacer, which enables writing and reading information on the nanoscale with variable letter sizes. Moreover, room temperature measurements indicate that such written structures could even persist room temperature.

O 85.6 Wed 18:15 Poster A

Optical properties of laser-excited metals in strong nonequilibrium — •Pascal D. Ndione[1], Sebastian T. Weber[1], Dirk O. Gericke[2], and Baerbel Rethfeld[1] — [1]Department of Physics and OPTIMAS Research Center, Technische Universitaet Kaiserslautern, 67653 Kaiserslautern, Germany — [2]Centre for Fusion, Space and Astrophysics, Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

Light-matter interactions in the femtosecond regime are of great importance for both our fundamental understanding and applications. The modification of optical properties is a key feature as reflectivity or transmissivity carry many informations about the correlated many body system. Short lasers pulses induce nonequilibrium in metals due to absorption of the photons' energy by the free electrons. On a time scale of a few tens to hundreds of femtoseconds after laser irradiation, the electrons thermalize to a Fermi distribution at an elevated temperature. We present here a model which keeps track of the band's occupation in metals triggered with optical photons. In addition, different approximations of the dielectric function are compared for metals driven far from equilibrium.

O 85.7 Wed 18:15 Poster A

Simulation of STM images and spectroscopy of molecules on metal surfaces: DFTB+ computational platform — •Seddigheh Nikipar[1], Dmitry A. Ryndyk[1,2], Bálint Aradi[2], Francesca Moresco[1], Gianaurelio Cuniberti[1], and Thomas Frauenheim[2] — [1]Institute for Materials Science and Center for Advancing Electronics Dresden, TU Dresden, Dresden, Germany — [2]Bremen Center for Computational Materials Science, Department of Physics, Universität Bremen, Bremen, Germany

We developed a theoretical and computational approach for simulations of STM images and spectroscopy, in particular of molecules on metal surfaces. We employed the DFT based atomistic tight-binding model (DFTB approach) combined with the Green function technique, which offers a framework to consider a tip, molecule and surface as one integrated system and taking into account the tip geometry. Besides, it captures the interference and interaction effects. This new computational approach can be applied for the investigation of finite-voltage effects and describe the higher molecular transport states. It allows to calculate the tunneling current between a tip and a molecule more precisely, and simulate quantitatively dI/dV maps and spectroscopy curves. We developed the extension of the DFTB+ computational package (dftbplus.org), which makes possible and convenient calculations for large-scale molecular nanosystems on metall surfaces. Our approach is quite fast due to the DFTB approximation and the effective MPI parallelization. The DFTB+ is free software and can be used at HPC clusters.

O 85.8 Wed 18:15 Poster A

simulation of surface assembly and diffusion — •zhichao huang and kai wu — College of Chemistry and Molecular Engineering, Peking University, Beijing, China

The complexity of the assembly of molecules on the surface makes there is no predictable method of molecular assembly on the surface. When the interaction between the substrate-molecule interaction and the molecular-molecular interaction is weak, the effect of the substrate on the surface assembly structure can be approximately neglected and the molecular-molecular interaction is described using molecular mechanics to achieve the molecular structure Predictive molecular assembly structure. At present, this method has been successfully simulated to obtain trimellitic acid and other organic small molecules of the assembly structure, and experimental observation of the assembly structure consistent.

O 85.9 Wed 18:15 Poster A

Increase of Porosity and Pore Size of Electrodeposited ZnO Films for Using Metal Complexes as Redox Shuttles in Dye-Sensitized Solar Cells — •Thi Hai Quyen Nguyen, Raffael Ruess, and Derck Schlettwein — IAP, JLU Giessen, Germany

Electrodeposited ZnO is an attractive alternative for the commonly used TiO_2 in dye-sensitized solar cells (DSSCs). Pores in such ZnO are typically narrow, making it difficult to use metal complexes as redox shuttles which worked well in TiO_2-based DSSCs. The present work is dedicated to an optimization of the porosity and pore size of ZnO. Porous ZnO films were prepared by electrodeposition in the presence of different structure directing agents (SDA) such as Eosin Y. The influence of the deposition time and the SDA-concentration was analysed. Furthermore, the combination of Eosin Y with other SDA was investigated. The films were studied by SEM, XRD, confocal Laser microscopy and profilometry. The internal surface of the films was determined by gas sorption and by electrochemical impedance spectroscopy. Sample porosity was determined from the amount of Zn in the films allowing to estimate the average pore size in the films. A combination of Eosin Y with a substituted derivative as SDA led to porous ZnO films with high stability and larger pore size compared to films prepared with Eosin Y only. Porous ZnO films could be obtained at less negative deposition potentials allowing increased control of growth parameters. The success of the present work was proven by photovoltaic characterization of test cells based on these new films providing easier diffusion of the large complexes through the ZnO pore structure.

O 86: Overview Talk: Claudia Felser

Time: Thursday 9:30–10:15 Location: HE 101

Invited Talk O 86.1 Thu 9:30 HE 101

Weyl Semimetals and beyond! — •Claudia Felser — Max Planck Institut Chemische Physik fester Stoffe

Topology a mathematical concept became recently a hot topic in condensed matter physics and materials science. One important criteria for the identification of the topological material is in the language of chemistry the inert pair effect of the s-electrons in heavy elements and the symmetry of the crystal structure. Beside of Weyl and Dirac new fermions can be identified compounds via linear and quadratic 3-, 6- and 8- band crossings stabilized by space group symmetries. Binary phoshides are the ideal material class for a systematic study of Dirac and Weyl physics. Weyl points, a new class of topological phases was also predicted in NbP, NbAs. TaP, MoP and WP2. In NbP microwires we have observed the chiral anomaly. NbP has served as a model system for the gravitational anomaly in astrophysics and WP2 for a hydrodynamic flow of electrons. MoP and WP2 show exceptional properties such as high conductivity (higher than copper), high mobilties and a high magneto-resistance effect. With thermal and magnetoelectric transport experiments, a transition from a hydrodynamic electron fluid below 15 K into a conventional metallic state at higher temperatures is observed. The hydrodynamic regime is characterized by a viscosity-induced dependence of the electrical resistivity on the square of the channel width that coincides with as strong violation of the Wiedemann-Franz law. In magnetic materials the Berry curvature and the classical AHE helps to identify interesting candidates such as in Co2YZ and in Mn3Sn.

O 87: Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures V

Organizers: Sabine Maier, FAU Erlangen-Nürnberg; Meike Stöhr, University of Groningen

(Synopsis provided with part I of this session)

Time: Thursday 10:30–13:00 Location: MA 004

Invited Talk O 87.1 Thu 10:30 MA 004

Molecular structures for conductance measurements — •Richard Berndt — Christian-Albrechts-Universität zu Kiel, D-24098 Kiel

Switching and spin effects in adsorbed molecules may be addressed by probing their conductances with low-temperature scanning tunneling microscopes. My talk will first cover results from molecules that are brought into ultrahigh vacuum with electrospray. This method is suitable for largish molecules and consequently a degree of complexity may be added to the molecules themselves. In addition, measurements will presented from sublimable molecules that are adsorbed through suitable molecular subunits serving as platforms.

This work was supported by SFBs 668 and 677.

O 87.2 Thu 11:00 MA 004

On-surface molecular synthesis of thermally unaccessible molecules by reactive landing electrospray ion beam deposition. — •Lukas Krumbein[1], Sabine Abb[1], Suman Sen[1], Klaus Kern[1,2], and Stephan Rauschenbach[1,3] — [1]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — [3]University of Oxford, Department of Chemistry, OX1 3TA Oxford, UK

On-surface molecular reactions have been in the focus of research due to their potential impact in molecular devices and for robust surface functionalization. Generally those reactions require thermal activation.

Alternatively electrospray ion beam deposition (ES-IBD) provides charged molecular beams for deposition at collision energies freely tunable in the range of 2eV-200eV. A surface collision at this energy is sufficient to drive on-surface reactions at room temperature.

Using the Reichardt's Dye molecule as a model systems we demonstrate equivalent on-surface reactions upon thermal annealing as well as hyperthermal surface collision. In particular we observe the formation of covalently linked dimers and (cyclo-) dehydrogenation including transition states not accessible by thermal annealing.

O 87.3 Thu 11:15 MA 004

Electrospray deposition of a Spoked Wheel molecule on bulk insulator surfaces in UHV — •Sebastian Scherb[1], Antoine Hinaut[1], Akimitsu Narita[2], Klaus Müllen[2], Sara Freund[1], Zhao Liu[1], Thilo Glatzel[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Max Planck Institute for Polymer Research, Mainz, Germany

Deposition of large, structurally complex molecules in UHV provides interesting prospects for applications in optoelectronics and molecular electronics. With increasing size, complexity or chemical reactivity deposition by thermal evaporation becomes challenging. A possible way to deposit such molecules in clean conditions is electrospray deposition. Since for the study of electronic properties of molecules decoupling from the surface is mandatory, deposition on insulator surfaces is necessary. In previous studies [1] triply fused porphyrin molecules were deposited on the KBr(001) surface, proving the capabilities of electro spray deposition for depositing organic molecules on bulk insulator.

Here, we report the deposition of a shape persistent polyphenylene Spoked Wheel molecule [2] onto KBr(001) using electrospray deposition in UHV. We show island growth on Au(111) and KBr(001) surfaces by ncAFM study in UHV at room temperature. We are further able to provide molecular resolution of islands, observing straight interdigitation of alkyl chains on the Au(111) surface and a tilting of the interdigitating alkyl chains on the KBr(001) surface.

[1] Hinaut, A. et al., Beilstein J. Nanotechnol. 6, 1927-1934 (2015). [2] Liu, Y. et al., J. Am. Chem. Soc. 138, 15539-15542 (2016).

O 87.4 Thu 11:30 MA 004

Self-assembly of synthetic peptides on surfaces — •Uta Schlickum[1,2], Sebastian Koslowski[1], Suman Sen[1], Xu Wu[1], Sabine Abb[1], Stephan Rauschenbach[1], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]Institut für Angewandte Physik, TU Braunschweig, 38106 Braunschweig, Germany — [3]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Peptides have outstanding intriguing functionalities determined by their self-assembled structures. We have investigated the self-assembly of peptides on surfaces to probe the interaction between specific amino acids at sub-molecular length scales. For these high resolution studies we deposited the peptides under ultrahigh vacuum conditions using an electrospray ion beam deposition source and transferred them in-situ into a low temperature scanning tunneling microscope. Our model systems of synthetic peptides consist of eight amino acids including only Arginine, Proline, and Tryptophan. Our results show, how tiny changes within simple peptide sequences drastically influence the self-assembly pattern due to the high conformational freedom of these molecular systems.

O 87.5 Thu 11:45 MA 004

Characterization and prediction of peptide structures on inorganic surfaces — •Dmitrii Maksimov, Carsten Baldauf, and Mariana Rossi — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Interfacing biological molecules with inorganic materials can give access to new technology that joins the versatile character of the biomolecular world with the robust electronic properties of inorganic materials. Peptides, for example, present a large degree of modularity, chemical versatility and conformational adaptability. However, their high degree of conformational freedom makes it a challenge to be able to predict structural motifs and understand the physics governing them. Here we address the structure-search problem by extending a first-principles genetic algorithm package that works on internal degrees of freedom [1] in order to include the position and orientation of molecules with respect to the surface. We show that energy differences between different conformations of the flexible ArgH^+ amino acid on Cu(111) show significant discrepancies when optimized with a force-field (tailored for peptide-surface interactions [2]) and with dispersion-corrected DFT. We further show that the excess charge of the protonated ArgH^+ is efficiently screened upon adsorption on metallic surfaces and that the Arg amino acid adopts a zwitterionic conformation on Cu(111) which considerably increases the molecular dipole parallel to the surface. [1] A. Supady, et al., JCIM 55, 2338 (2015) [2] F. Emami, et al., Chem. Mat. 26, 2647 (2014).

O 87.6 Thu 12:00 MA 004

Electrospray deposition of structurally complex molecules revealed by atomic force microscopy — •Antoine Hinaut[1], Tobias Meier[1], Remy Pawlak[1], Sara Freund[1], Klaus Müllen[2], Silvio Decurtins[3], Thilo Glatzel[1], Akimitsu Narita[2], Shi-Xia Liu[3], and Ernst Meyer[1] — [1]Dep. of Physics, Univ. of Basel, Switzerland. — [2]MPI for Polymer Research, Mainz, Germany — [3]Dep. of Chemistry and Biochemistry, Univ. of Bern, Switzerland

Increasing complexity and functionalization of molecular species studied in ultra high vacuum is actually mainly limited by the deposition technique. We used our electrospray deposition setup[1,2], to introduce two molecular species in ultra high vacuum. The first molecule, based on large aromatic core, includes six long alkyl chains. Assemblies on the Au(111) surface both at room temperature with ncAFM and at low temperature with AFM/STM are observed. Their formation is directed by alkyl-alkyl interaction and is also influenced by the measurement temperature. The second species is a fused electron donor-acceptor molecule. Measurement on the Au(111) surface at low temperature AFM/STM shows small island formation directed by H-bond interaction. In both cases we reach cleanliness levels compatible with high-resolution CO functionalized tip AFM measurements and show the intact chemical structures after electrospray deposition. Therefore our setup combined with high resolution scanning probe measurements allows investigation of more complex compounds with attractive properties. [1] Hinaut et al., BJNano, 2015, 6, 1927-1934. [2] Hinaut et al., submitted to Nanoscale.

O 87.7 Thu 12:15 MA 004

STM studies of functional platform adlayers on Au(111) surfaces — •Talina Rusch[1], Roland Löw[2], Alexander Schlimm[3], Felix Tuczek[3], Rainer Herges[2], and Olaf M. Magnussen[1] — [1]Institute of Experimental and Applied Physics, Kiel University, Germany — [2]Otto Diels Institute of Organic Chemistry, Kiel University — [3]Institute of Inorganic Chemistry, Kiel University

The functionalization of surfaces by self-assembled monolayers is of great interest in nanoscience. We have introduced the so called platform approach, where molecular platforms of Triazatriangulenium (TATA) [1, 2, 3] ions are employed for attaching freestanding functional units to metal surfaces. These platforms provide a well-defined lateral and vertical molecular architecture and the steric demand is controlled by different alkyl side chains. Here, detailed STM studies on different adsorbate layers of TATA derivatives are presented. Specifically, we will discuss the structure of mixed adlayers consisting of two different TATA derivatives, one where the attached azobenzene is fully conjugated and one where it is isolated. We found that those TATA derivatives are perfectly mixable and randomly distributed on the Au(111) surface. Furthermore, we will present direct STM observations of the photoswitching in new azobenzene functionalized TATA adsorbate layers.This work was supported by the Deutsche Forschungsgemeinschaft via SFB 677 "Function by switching". [1] B. Baisch et al., J. Am. Chem. Soc. 131 (2009) 442 - 443. [2] S. Kuhn et al., Phys. Chem. Chem. Phys. 12 (2010) 4481 - 4487. [3] J. Kubitschke et al., Eur. J. Org. Chem. 2010 (2010) 5041 - 5055.

O 87.8 Thu 12:30 MA 004

Supramolecular nanopatterns of arylene-alkynylenes on HOPG: Insights from STM — •Stefan-S. Jester — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany.

Arylene-alkynylenes with sufficiently long alkyl/alkoxy side chains form self-assembled monolayers at the solid/liquid interface on graphite (HOPG). 2D crystal engineering relates the size and shape of the molecules with the lattice constants and symmetries of these supramolecular nanopatterns. Scanning tunneling microscopy provides a submolecularly resolved insight. Tesselation concepts can be applied to design cocrystals (e.g., of triangles and hexagons), and the symmetry mismatch between molecule and the substrate lattice leads to complex superstructures (e.g., observed for pentagons).[1] The hierarchical formation of frustrated superstructures is observed for C_{3v} symmetric molecules, but still difficult to predict.[2] Thereby, not only the number of alkoxy side chains per molecule, but also the substitution pattern is crucial for the periodic pattern formation, as we show for molecular spoked wheels.[3] [1] S.-S. Jester, E. Sigmund, S. Höger *J. Am. Chem. Soc.* **2011**, *133*, 11062; [2] S.-S. Jester, E. Sigmund, L. Röck, S. Höger *Angew. Chem. Int. Ed.* **2012**, *51*, 8555; [3] A. Idelson, C. Sterzenbach, S.-S. Jester, C. Tschierske, U. Baumeister, S. Höger *J. Am. Chem. Soc.* **2017**, *139*, 4429.

O 87.9 Thu 12:45 MA 004

Two switchable rotaxanes operating in multilayers on solid support investigated by XPS and NEXAFS — •Thomas Heinrich[1,2], Henrik Hupatz[2], Andreas Lippitz[1], Christoph A. Schalley[2], and Wolfgang E. S. Unger[1] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), 6.1 Surface Analysis and Interfacial Chemistry, Unter den Eichen 44-46, 12205 Berlin — [2]Institut für Chemie und Biochemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin, Germany

Interfaces provide the structural basis for function as, for example, encountered in nature in the membrane-embedded photosystem or in technology in solar cells. Synthetic functional multilayers of molecules cooperating in a coupled manner can be fabricated on surfaces through layer-by-layer self-assembly. Ordered arrays of stimuli-responsive rotaxanes undergoing well-controlled axle shuttling are excellent candidates for coupled mechanical motion. The present work demonstrates the successful deposition of ordered mono- and multilayers of chemically and photochemically switchable rotaxanes on gold surfaces. Two substrates are investigated - silicon and gold. Of these materials, only gold showed to be suitable for the development of highly preferential oriented rotaxane layers. XPS indicates for both substrates that our layer-by-layer approach worked and a layer growth with every deposition step is present. NEXAFS showed that both stimuli cause an increase of the multilayer's preferential orientation and that the switching is reversible. However, these effects are only observed for the multilayers on gold surfaces.

O 88: Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00 Location: MA 005

Invited Talk O 88.1 Thu 10:30 MA 005

Syngas reactions on metal surfaces studied using scaling-relation-based kinetic Monte Carlo — •Mie Andersen — Theoretical Chemistry, Technische Universität München, Germany

The complexity of catalytic reactions on surfaces calls for efficient means of estimating adsorption energies and reaction barriers, which are required input for a microkinetic model. One commonly used approach is to employ scaling relations [1], which are linear relations between the adsorption energies of atomic and molecular species on various (typically metal) surfaces, in combination with simple rate equations for the catalytic activity based on the mean-field approximation (MFA). In my talk, I will demonstrate the prospects of instead combining scaling relations with kinetic Monte Carlo simulations, which allow for predicting the catalytic activity while taking into account spatial correlations in the distribution of the adsorbates on the surface. For the specific case of methane synthesis from syngas on stepped metal surfaces, I demonstrate that MFA models may overestimate the catalytic activity of metal catalysts by several orders of magnitude due to the neglect of spatial correlations [2]. Finally, I will discuss recent and ongoing work aimed at (i) overcoming challenges related to a large disparity in the timescales of the surface processes, (ii) accounting for lateral interactions between the adsorbates, and (iii) dealing with more complex reaction networks such as the synthesis of higher alcohols on metal catalysts.

[1] F. Abild-Pedersen, Catal. Today **272**, 6 (2016)
[2] M. Andersen *et al.*, J. Chem. Phys. **147**, 152705 (2017)

Invited Talk O 88.2 Thu 11:00 MA 005

Catalytic reactivity of binary alloys studied by field emission techniques — •Cédric Barroo, Yannick De Decker, Luc Jacobs, and Thierry Visart de Bocarmé — Université Libre de Bruxelles

Field emission techniques are well-suited to study the dynamics of catalytic reactions occurring at the surface of a nanosized metal tip which represents a good model of a single catalytic nanoparticle. Here, field ion microscopy (FIM) is used to determine the structure of the alloys, and field emission microscopy (FEM) to study the dynamics of reactions during the ongoing processes. We studied the NO2+H2 reaction on Pt-Rh. Previous experiments on Pt and Rh proved the presence and robustness of nonlinear dynamics, such as self-sustained periodic oscillations and propagation of chemical waves. On the Pt-Rh alloy, non-linear behaviors were observed: the characteristics of the oscillations lie between the features on pure Pt and Rh. The existence of periodic oscillations during the NO2+H2 reaction on Pt, Rh and Pt-Rh samples suggest that the mechanism behind the occurrence of those oscillations is robust and seems to mostly depend on the reaction itself and less on the nature of the substrate. The mechanism of reaction is discussed. We also studied the N2O+H2 reaction on Au-Ag, where N2O serves as a supplier of O(ads) since the ability to supply adsorbed oxygen is the key for activity/selectivity on gold surfaces. The reactive behavior can be observed via the appearance of new field emission patterns. These results prove the relevance of field emission techniques to study the catalytic activity of alloys.

Invited Talk O 88.3 Thu 11:30 MA 005

Imaging spin polarization and orbital character at surfaces: from the Rashba effect to topological Fermi arcs — •H. Bentmann, H. Maass, C.-H. Min, and F. Reinert — Experimentelle

Physik VII, Universität Würzburg

With the discovery of topological quantum states in solids, surface states have emerged from a niche phenomenon to a central concept in modern surface science and condensed matter physics, in general. Protected surface states with unconventional spin textures in momentum space are the hallmark of topological phases of matter being driven by spin-orbit interaction. Here, we shall present systematic spin- and angle-resolved photoemission investigations of strongly spin-orbit coupled surface states [1-3], spanning the range from the Rashba effect over topological insulators to the exotic Fermi arcs in Weyl semimetals. We will show that these experiments -based on a careful consideration of the photoemission transition-matrix-element [1]- are able to yield a detailed insight into the momentum-dependent structure of the surface-state wave function, in terms of spin polarization [1], orbital character [2], and bulk penetration [3]. For the example of the Weyl semimetal TaP, we will discuss how the measured orbital character across the Fermi surface reflects the non-trivial topology of the Fermi-arc surface states.

[1] HB et al., Phys. Rev. Lett. 119, 106401 (2017).
[2] H. Maass, HB, et al., Nature Commun. 7, 11621 (2016).
[3] C. Seibel, HB, et al., Phys. Rev. Lett. 114, 066802 (2015).

Invited Talk O 88.4 Thu 12:00 MA 005

Tuning optoelectronic properties of silicon quantum dots via surface chemistry — •Mita Dasog[1,2,3], Jonathan G. C. Veinot[2], and Nathan S. Lewis[3] — [1]Department of Chemistry, Dalhousie University, Halifax, NS, Canada — [2]Department of Chemistry, University of Alberta, Edmonton, AB, Canada — [3]Division of Chemistry and Chemistry Engineering, California Institute of Technology, Pasadena, CA, United States

Over the last thirty years, quantum dots have become an indispensable tool for optoelectronic applications. The optical properties of colloidal quantum dots can be tuned through their size and shape. Among them silicon quantum dots (Si-QDs) have attracted attention due to their natural abundance and bio-compatibility. While few reports exist on size dependent emission from Si-QDs, the vast majority of them defy quantum confinement effect. In this talk, surface chemistry methodologies and luminescence in Si-QDs originating from surface states will be discussed. It was discovered that the emission can be tuned across the visible spectrum by changing the surface groups. The blue-to-green emission originating from oxynitride defect-states have shorter excited lifetimes and higher emission quantum yields compared to the bandgap emission in Si-QDs and the yellow-to-orange emission can originate from suboxide defect-states and have longer excited lifetimes and lower emission quantum yields. The Si-QDs can be further functionalized with surface molecules for bioimaging and explosives sensing.

Invited Talk O 88.5 Thu 12:30 MA 005

Carbon Dioxide Activation at Metal-Oxide Surfaces: A Compressed-Sensing Analysis — •Aliaksei Mazheika[1], Yang-gang Wang[1], Rosendo Valero[2], Francesc Illas[2], Runhai Ouyang[1], Luca M. Ghiringhelli[1], Sergey V. Levchenko[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin 14195, Germany — [2]Universitat de Barcelona, Barcelona 08007, Spain

Conversion of carbon dioxide (CO$_2$) to hydrocarbon fuels would allow for a sustainable energy utilization. CO$_2$ is a stable molecule, which requires an activation prior to conversion. It can be activated by adsorption on a solid surface. In this work, we employ compressed-sensing (SISSO) [1] and subgroup-discovery [2] approaches to find physically interpretable *ab initio* descriptors for energy and structure of CO$_2$ adsorbed at binary and ternary oxide surfaces. The descriptors include only properties of involved atomic species, bulk materials, and clean surfaces. We show that, contrary to the standard understanding, the O-C-O bending angle does not correlate well with the charge transferred to CO$_2$ for the whole data set. However, the subgroup discovery identifies a subset of surfaces for which this correlation is accurate. This subset is characterized by a more ionic character of the bonding between surface cations and O. Applying SISSO to this and the remaining subset independently, we obtain more accurate descriptors than for the whole data set.

[1] R. Ouyang *et al.*, arXiv:1710.03319
[2] B. Goldsmith *et al.*, New J. Phys. **19** 013031 (2017)

O 89: Oxide and Insulator Surfaces: Structure, Epitaxy and Growth I

Time: Thursday 10:30–13:00 Location: MA 041

O 89.1 Thu 10:30 MA 041

High resolution imaging of ultrathin ZnO layers epitaxially grown on Ag(111) using scanning tunneling hydrogen microscopy — •Shuyi Liu[1], Akitoshi Shiotari[2], Delroy Baugh[3], Martin Wolf[1], and Takashi Kumagai[1] — [1]Department of Physical Chemistry, Fritz-Haber Institute of the Max-Planck Society, Germany. — [2]Department of Advanced Materials Science, Japan. — [3]Department of Chemistry & Biochemistry, University of California, USA.

Ultra-high resolution imaging with a molecular STM/AFM junction has attracted increasing attention as a fascinating tool to resolve submolecular structures of adsorbates [1]. Termirow et al. found that molecular hydrogen in an STM junction can enhance the image contrast of planar organic molecules and proposed the idea of scanning tunneling hydrogen microscopy (STHM)[2]. However, the conductivity and mechanical property of the hydrogen junction are imperfectly understood. We apply STHM to image ultrathin ZnO layers epitaxially grown on Ag(111) and the atomic resolution can be obtained in a reproducible manner. We performed the gap distance-dependent conductance measurement and force spectroscopy using STM/AFM, revealing that the junction consists of multiple hydrogen molecules and the enhanced resolution can be achieved at a specific tip-surface distance. A simplified model with two hydrogen molecules in the junction reproduced the distance dependent conductance, force curve and enhanced imaging of ZnO. [1]P. Jelínek J. Phys.: Condens. Matter 29 343002 (2017). [2]R. Temirov et al. New J. Phys. 10, 053012 (2008).

O 89.2 Thu 10:45 MA 041

VO$_2$ growth on TiO$_2$(110) using atomic oxygen — •Simon Fischer, Jens Falta, Jan Ingo Flege, and Jon-Olaf Krisponeit — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

VO$_2$ thin film growth is of interest for switching devices and sensorics because it exhibits a temperature-induced metal-insulator transition. This is accompanied by a structural change between a monoclinic insulating phase and a rutile metallic phase, allowing for tuning the transition temperature by choice of the substrate: TiO$_2$(110) as a substrate applies in-plane tensile strain to the rutile *c*-axis and thus increases the transition temperature, favoring the monoclinic phase.

VO$_2$ growth is challenging in terms of achieving the correct stoichiometry, which is why we used an activated oxygen source. We examined the deposition of 5 to 10 nm of VO$_2$ on TiO$_2$(110) in-situ using LEEM and LEED. Additionally, from XPS measurements we determined the stoichiometry by analyzing the chemical shift of the V2$p_{3/2}$ peak and we estimated the film thickness from the attenuation of the substrate peak. High doses of atomic oxygen enable the formation of V$_2$O$_5$ domains of random azimuthal orientation, while lower doses lead to oxygen vacancies that impair transition characteristics as observed in ex-situ measurements.

Financial support from the DFG is acknowledged.

O 89.3 Thu 11:00 MA 041

Pulsed laser deposition of In$_2$O$_3$ thin films on YSZ(111) — •Michele Riva[1], Giada Franceschi[1], Jakob Hofinger[1], Margareta Wagner[1,2], and Ulrike Diebold[1] — [1]IAP, TU Wien — [2]FAU Erlangen-Nürnberg

In$_2$O$_3$ is a wide band-gap, transparent conductive oxide whose applications include optoelectronics, gas sensing, and catalytic fuel production. In all these applications In$_2$O$_3$ surfaces and their nanoscale properties play a key role, and atomic-scale investigations to unravel such properties require suitable single-crystalline model systems. However, In$_2$O$_3$ single crystals are not commercially available, and synthetically grown ones are usually very small. While this is not critical for scanning probe techniques, area-averaging techniques such as TPD and XPS require larger samples. To this purpose, we have grown well-ordered and atomically flat In$_2$O$_3$(111) thin films - with a thickness of a few hundred nanometers - onto YSZ(111) substrates by PLD. Their structure, chemical composition and morphology were characterized by RHEED, LEED, XRD, XPS, AFM, and STM. By optimizing the growth parameters, we could obtain In_2O_3(111) films exhibiting properties comparable to the best single crystals available, exhibiting atomically-flat terraces a few hundred nanometers wide, separated by monoatomic steps. The films behave like In_2O_3 single crystals, down to the atomic scale, and thus allow the combination of atomic-scale surface-science analysis and the investigation of, e.g., the electronic structure and the reactivity of their surfaces via area averaging spectroscopic techniques.

O 89.4 Thu 11:15 MA 041

The stability of ultra-thin ZrO_2 films on a metallic substrate: a challenge for DFT? — Wernfried Mayr-Schmölzer, Jakub Planer, Tobias Hruby, Florian Mittendorfer, and •Josef Redinger — Institute of Applied Physics and Center for Computational Materials Science, TU Vienna, Wiedner Hauptstrasse 8-10/134, 1040 Vienna, Austria

At first DFT calculations for bulk ZrO_2 are performed to assess the accuracy of semi-local, vdW corrected and hybrid functionals as compared to a many-body approach, ACFDT-RPA. Whereas all the functionals reproduce the experimental order of stabilities of known phases, the relative stability of two additionally found meta-stable phases with comparable energies depends on the functional used. For ultra-thin films on metals as grown both on Pt(111) [1] and Rh(111) [2], we investigate the structural stabilities of a suggested tri-layer O-Zr-O film on both substrates. The DFT calculations show that such O-Zr-O trilayers are quite strained on both metals, but they behave differently on Pt or Rh. Obviously, for Rh the tensile stress can be compensated by O-Rh bonds at the interface while this is not working for Pt. For Pt the stress leads to a heavily corrugated O-Zr-O layer not witnessed in experiment. Even the recently developed most advanced SCAN meta-GGA functional, which matches well with our ACFDT-RPA benchmark for bulk ZrO_2, does not cure the problem.

[1] M. Antlanger, et. al., PRB86, 035451 (2012)

[2] P. Lackner and M. Schmid, TU Vienna, work in progress (2017)

O 89.5 Thu 11:30 MA 041

Relaxation effects in $VO_2/TiO_2(001)$ films — •Jon-Olaf Krisponeit[1], Simon Fischer[1], Sven Esser[2,3], Vasily Moshnyaga[3], Jan Ingo Flege[1], and Jens Falta[1] — [1]Institut für Festkörperphysik, Universität Bremen, 28359 Bremen, Germany — [2]Experimentalphysik VI, Universität Augsburg, 86159 Augsburg, Germany — [3]1. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Bulk vanadium dioxide (VO_2) exhibits a metal-insulator transition at 340 K. On TiO_2(001) substrates, the tensile in-plane stress can be utilized for a reduction of T_{MI} to room temperature due to the compression of the out-of-plane rutile c-axis of VO_2.

Aiming for such epitaxial VO_2/TiO_2(001) films under high coherent strain, potential relaxation effects annihilating stress and/or modifying surfaces and interfaces should be taken into account. Films were prepared by reactive molecular beam epitaxy and metal-organic aerosol deposition. Structural and morphological properties were analyzed by low-energy electron microscopy and diffraction as well as scanning probe microscopy. We discuss three distinct relaxation effects: (i) surface facetting, (ii) the formation of a misfit dislocation network, and (iii) topographic buckling and even crack patterns for thick films.

Support by the Institutional Strategy of the University of Bremen funded by the German Excellence Initiative is acknowledged.

O 89.6 Thu 11:45 MA 041

Strain and ordering effects of ultrathin epitaxial ferrite films on $SrTiO_3$(001) — •Jari Rodewald, Tabea Nordmann, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Ultrathin epitaxial ferrite films as $NiFe_2O_4$ or $CoFe_2O_4$ are in the focus of spintronics since both materials are insulating and ferrimagnetic. Thus, they are well-suited to be used as spin filters due to spin dependent tunneling barrier. Here, the homogeneity of the films is essential to form tunneling barriers. Furthermore, the cation ordering on the different sublattices of the inverse spinel structure determines the magnetic properties of the ferrite films which is crucial for the performance as a spin filter. Therefore, the formation of ferrite films has to be carefully controlled if high quality devices are aimed for.

Hence, in this work ultrathin ferrite films of different thicknesses are prepared via reactive molecular beam epitaxy (RMBE) on $SrTiO_3$(001). In order to investigate structural strain and ordering effects in the films, synchrotron radiation grazing incidence x-ray diffraction (SR-GIXRD) experiments are performed. The chemical composition and structural ordering at the surface are investigated by x-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED), respectively. Magnetic properties are characterized via superconducting quantum interference device (SQUID) magnetometry.

O 89.7 Thu 12:00 MA 041

A structure analysis of the $BaTiO_3$-derived oxide quasicrystal in physical and internal space — •Sebastian Schenk[1], Stefan Förster[1], René Hammer[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 $BaTiO_3$-derived and $SrTiO_3$-derived 2-dimensional oxide quasicrystals (OQC) with 12-fold symmetry have been discovered on Pt(111) substrates [1,2]. Both OQCs exhibit a Niizeki-Gähler tiling which is composed by quadratic, triangular, and rhombic elements of equal side length. This tiling can be derived mathematically from cutting a periodic hyperhexagonal structure in the four-dimensional space and project it onto two dimensions, the so-called physical space. Here, we present a detailed analysis of the tiling characteristics as derived from atomically-resolved STM images which represent the physical space dimension. Not only the tiling frequency, but also their orientational distribution is determined to unravel the impact of the underlying periodic substrate to the OQC tiling. Additional information is gained from lifting the atomic coordinates into the four-dimensional hyperspace for a subsequent study of the internal space projection.

[1] S. Förster et al., Nature **502**, 215 (2013)

[2] S. Schenk et al., J. Phys.: Condens. Matter **29**, 134002 (2017)

O 89.8 Thu 12:15 MA 041

In-situ investigations of pulsed-laser-deposited Sr-doped lanthanum manganite thin films — •Giada Franceschi, Michele Riva, Michael Schmid, and Ulrike Diebold — Inst. Appl. Phys., TU Wien, Wiedner Haupstrasse 8-10, 1040 Wien, Austria

Sr-doped lanthanum manganite ($La_{0.8}Sr_{0.2}MnO_3$, or LSM) is a widely used material as a cathode in solid oxide fuel cells, and atomic-scale understanding of the reactions occurring at its surface is interesting from both fundamental and application-driven points of view. Atomic-scale investigations require a well-defined and well-ordered system, but LSM single-crystals are not available commercially. In the present contribution, I will show our efforts towards the establishment of a model system for LSM, in the form of a thin, pulsed-laser-deposited film onto $SrTiO_3$(110) substrates.

Combination of pulsed laser deposition with in situ surface sensitive techniques (STM, LEED, XPS, LEIS) allows to controllably tune the surface composition, and establish a relation with its structure.

O 89.9 Thu 12:30 MA 041

Formation of Transition-Metal-Oxide Chains on Ir(110) — •Tilman Kisslinger[1], Robert Jacob[1], Josef Redinger[2], M. Alexander Schneider[1], and Lutz Hammer[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen–Nürnberg, D–91058 Erlangen, Germany — [2]Institut für Angewandte Physik & CMS, TU Wien

Evaporation of 0.5 ML of the 3d transition metals (TM's) Co, Ni and Fe at 100 K onto the unreconstructed Ir(110)–(1×1) surface and oxidation at 920 K leads to the formation of large domains of monatomic chains that are separated by two surface lattice parameters in [001] direction as revealed by STM. For all TM = Co, Ni, Fe similar LEED I(V)–spectra are found indicating the same surface structure. This structure was quantitatively determined for the case of TM = Co ($R_P = 0.117$) revealing CoO_2 stoichiometry. The TM sits at hollow sites of the first Ir layer and is surrounded by four oxygen atoms being threefold coordinated towards two 3d–TM and one Ir atom. All structural parameters are in close agreement to independently conducted DFT calculations. The structural motif of this system is rather similar to the one found on Ir(100) [1]. However, on Ir(110) the TMO_2 chains do not induce a missing–row reconstruction and thus adsorption sites for possible reaction partners are blocked. This modifies e.g. their reactivity and manifests itself in the higher temperature of 420 K necessary for hydrogen–reduction of the phase on Ir(110), compared to 330 K on Ir(100) [2].

[1]: Ferstl *et al.*, Phys. Rev. Lett. **117**, 4 (2016)

[2]: Ferstl *et al.*, Phys. Rev. B **96**, 085407 (2017)

O 89.10 Thu 12:45 MA 041

A mesoscopic view on ultra-thin germania films on Ru(0001) — •Alexander Fuhrich[1], Thomas Schmidt[1], Dietrich Menzel[1,2], and Hans-Joachim Freund[1] — [1]Department of Chemical Physics, Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany — [2]Physik-Department E20, Technische Universität München, Garching, Germany

The silica bi-layer system on Ru(0001) has been intensely studied by different techniques [1,2]. However, the modification of these ultrathin films by using germanium instead of silicon offers many interesting opportunities for catalysis and the understanding of the growth of ultrathin semiconductor oxides on metal single crystals. Using spectromicroscopy (LEEM, LEED, XPEEM and XPS), we studied the growth and structures of ultra-thin germania supported on Ru(0001). The growth of germanium and germania on Ru(0001) was observed in real-time and in-situ at mesoscopic scale. The morphology and structure of the Germania films will be discussed in dependence on preparation parameters . The presence of oxygen reduces the diffusion of germanium on Ru(0001). Though deposited in UHV, germanium is partially oxidized by oxygen pre-covered on the Ru surface. The fully oxidized Germania film exhibits a 2x2 structure on Ru(0001) and, up to now, no evidence was found for a vitreous germania phase on Ru(0001) like it is the case for silica.

References 1. H.W. Klemm, G. Peschel, E. Madej, A. Fuhrich, M. Timm, D. Menzel, Th. Schmidt, H.-J. Freund, Surf. Sci. 646, 45-51 (2016) 2. S. Shaikhutdinov, H.-J. Freund, Adv. Mater 25, 49-67 (2013)

O 90: Electronic structure of surfaces: Spectroscopy, surface states IV

Time: Thursday 10:30–13:00 Location: MA 042

O 90.1 Thu 10:30 MA 042

Mahan cone backfolding in Phthalocyanine overlayers on Au(111) — •Benito Arnoldi, Dominik Jungkenn, Johannes Seidel, Johannes Stöckl, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics, TU Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

Here, we extend our previous study of the spin-polarization of Mahan cone transitions of bare noble metals to metal-organic interfaces. For the latter material system, the long range order of the molecular film leads to clear back-folding of the central Mahan cone, i.e., to a scattering of substrate electrons at the molecular films. We employ spin and angle resolved laser ARPES with linear polarized light and 6eV photons to gain insight into the spin-polarization of the backfolded Mahan cones for monolayer films of CuPc and H2Pc on Au(111). For both molecular adsorbates, we observe a clear spin-polarization for the main Mahan cones, but not for the backfolded cones. A comparison of our results with previous findings for the Mahan cone spin polarization for the bare Au(111) surface and Bi/Au(111) interfaces will allow us to gain insight into spin-dependent scattering and spin-dependent back-folding of substrate bands at adsorbate films.

O 90.2 Thu 10:45 MA 042

Manipulating electron scattering resonances in graphene — •Maxim Krivenkov, Dmitry Marchenko, Jaime Sánchez-Barriga, Oliver Rader, and Andrei Varykhalov — Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Str. 15, D-12489 Berlin, Germany

Scattering resonances were recently predicted to exist above the vacuum level of two-dimensional (2D) materials [1]. These resonances influence transmission of low-energetic electrons and should appear in photoemission experiments as strongly dispersive features of suppressed intensity. We were able to observe and systematically study these states in graphene by using angle-resolved photoemission spectroscopy. To investigate whether the resonances can be manipulated we explored three routes: growth of graphene on chemically diverse substrates - Ir(111), Bi/Ir, and Ni(111), enhancement of superlattice potential by Ir nanodots [2] and switching of hybridization type in graphene from sp^2 to sp^3 by hydrogenation. While strength of the chemical interaction with the substrate had almost no effect on the dispersion of the resonances, their energy varies with the magnitude of charge transfer from/to graphene. In contrast, deposition of superlattice of Ir nanodots as well as hydrogenation of graphene eliminate the resonances completely. Our results provide the ways of tuning optoelectronic properties of 2D materials with a graphene-like structure.

[1] V. U. Nazarov et al., Phys. Rev. B 87, 041405(R) (2013);

[2] M. Krivenkov et al., Appl. Phys. Lett. 111, 161605 (2017).

O 90.3 Thu 11:00 MA 042

The nature of surface conductivity in samarium hexaboride — Peter Hlawenka[1], Konrad Siemensmeyer[1], Eugen Weschke[1], Jaime Sánchez-Barriga[1], Andrei Varykhalov[1], Natalya Shitsevalova[2], Slavomir Gabáni[3], Karol Flachbart[3], Oliver Rader[1], and •Emile Rienks[4,5] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]National Academy of Sciences of Ukraine, Kiev, Ukraine — [3]Slovak Academy of Sciences, Košice, Slovakia — [4]Technische Universität Dresden, Dresden, Germany — [5]IFW Dresden, Dreden, Germany

The prediction that Kondo insulators could be topologically non-trivial renewed interest in SmB$_6$, a material that already earned a reputation as the first mixed valence system and Kondo insulator. Dzero et al.'s proposal [1] connects two of the most topical fields in solid state research: Topological insulators and strongly correlated materials. In addition, robust surface conductivity —inherent to a topological insulator— would elegantly explain SmB$_6$'s anomalous transport properties. The notion that samarium hexaboride is a topological Kondo insulator is seemingly confirmed by recent experiments: It is found to be a surface-only conductor at low temperature and surface states have been found at the expected locations [2]. In this talk we will present crucial new insights from high-resolution angle-resolved photoemission spectroscopy [3] and discuss the implications.

[1] M. Dzero, et al., Phys. Rev. Lett., 104 (2010) 106408. [2] J. W. Allen, Phil. Mag. 96 (2016) 3227. [3] First results: P. Hlawenka et al., ArXiv: 1502.01542v1.

O 90.4 Thu 11:15 MA 042

Spin-polarization of the two-dimensional electron gas at CaTiO$_3$ film surfaces — •Eduardo B. Guedes[1,2], Stefan Muff[1,2], Milan Radovic[2,3], and J. Hugo Dil[1,3] — [1]Institut de Physique, Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland — [2]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen, Switzerland — [3]SwissFel, Paul Scherrer Institut, 5232 Villigen, Switzerland

The perovskite CaTiO$_3$ was recently added to the group of oxides hosting a metallic surface state [1], which in this case consists exclusively of 2-dimensional electron gas (2DEG). We investigated films of CaTiO$_3$ grown by pulsed laser deposition by means of spin- and angle-resolved photoelectron spectroscopy (SARPES). Our results show that the surface state is clearly split into two bands, which present spin polarization consistent with a Rashba-like splitting. Further, possible spin-interference effects [2] are also seen in the spectra, and different scenarios for the role of spin in dipole selection rules will be discussed.

References:

[1] S. Muff et al., Observation of a two-dimensional electron gas at CaTiO$_3$ film surfaces, Appl. Surf. Sci. (2017), http://dx.doi.org/10.1016/j.apsusc.2017.05.229.

[2] U. Heinzmann and J. H. Dil, J. Phys.: Condens. Matter 24, 173001 (2012).

O 90.5 Thu 11:30 MA 042

Origin of Surface States in ZrSiS and related compounds — •Andreas Topp[1], Raquel Queiroz[1,2], Leslie M. Schoop[1,3], and Christian R. Ast[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, DEU-70569 — [2]Weizmann Insitute of Science, Rehovot, ISR-7610001 — [3]Department of Chemistry, Princeton University, Princeton, USA-08544

Three-dimensional Dirac semimetals, which accomodate massless Dirac and Weyl fermions, show exotic physical properties, e.g. an extremly high mobility and giant magnetoresistance. Compounds that comprise nonsymmorphic symmetries are especially interesting as the band crossings that are protected by the symmetry, are not effected by SOC. ZrSiS, hosting a square lattice of Si atoms, has shown normal, as well as, nonsymmorphically protected 3D Dirac crossings at and close to the Fermi level [1]. ARPES measurements showed additional surface states crossing the bulk bands, which do not fit in the current scheme of surface states. Here, we analyze their origin by comparing ARPES data with DFT and tight-binding calculations. We present the idea of a selective symmetry breaking through the surface that lifts the nonsymmorphic degeneracy at the X point and leads to the formation of these surface states.

[1] L. M. Schoop *et al.*, Nat. Comm. 7, 11696 (2016).

O 90.6 Thu 11:45 MA 042

Manipulation of the 2DEG at Titanates Surfaces — •Stefan Muff[1,2], Nicolas Pilet[2], Mauro Fanciulli[1,2], Andrew P. Weber[1,2], Zoran Ristic[2], Zhiming Wang[2,3], Eduardo Bonini Guedes[1,2], Nicholas Plumb[2], Milan Radovic[2], and Hugo Dil[1,2] — [1]Institut de Physique, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne — [2]Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen — [3]Department of Quantum Matter Physics, University of Geneva, CH-1211 Geneva

In this talk, different ways to manipulate the 2DEG of the titanates (001) surface are presented. Crystalline surfaces and films grown by pulsed laser deposition (PLD) are studied by the help of angle-resolved photoelectron spectroscopy (ARPES) to explore the changes in the orbital ordering and band filling of the studied compounds.

In vicinal $\mathrm{SrTiO_3}$ and films of $\mathrm{CaTiO_3}$, the tetragonal distortion of the $\mathrm{TiO_6}$ octahedra is altered due to the changed surface free energy and chemical strain respectively. With the strong dependence of the formation of the titanates 2DEG on the surface crystal structure, the change in distortion directly affects the energy scale of the orbital ordering of the Ti 3d states, that form the 2DEG of these two systems. For thin films of $\mathrm{SrTiO_3}$ grown by PLD, the different type of growth defects and the surface potential landscape are responsible for an observed change in band filling of the 2DEG. The presented results show different ways to manipulate the 2DEG of titanates surfaces and open new paths to engineer the 2DEG and consequently the transport properties of the studied and closely related systems.

O 90.7 Thu 12:00 MA 042

Electronic structure of the non-polar GaN($10\bar{1}0$) surface — Martin Franz[1], Stephan Appelfeller[1], Holger Eisele[1], Philipp Ebert[2], and •Mario Dähne[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin — [2]Peter Grünberg Institut, Forschungszentrum Jülich

The non-polar GaN($10\bar{1}0$) surface, the so-called m-plane, plays an important role in nitride devices, e.g. as the predominant sidewall facet of nanowires or as a promising growth substrate for a reduction of polarization fields. However, detailed experimental results on the nature of the GaN($10\bar{1}0$) surface states are still scarce.

In this work, the electronic structure of the *n*-GaN($10\bar{1}0$) cleavage surface was studied using angle-resolved photoelectron spectroscopy at BESSY. The bulk valence bands and the filled nitrogen-related surface-state band could be clearly identified, allowing to determine the dispersion of the surface-state band and to derive the effective masses for both the bulk and surface valence bands. In addition, the position of the Fermi level within the band gap was determined at around 2.3 eV above the valence-band maximum, corresponding to the energetic position of the minimum of the empty gallium-related surface-state band, in nice agreement with recent theoretical results [1].

This work was supported by the DFG, Sfb 787, TP A4.

[1] L. Lymperakis, P.H. Weidlich, H. Eisele, M. Schnedler, J.-P. Nys, B. Grandidier, D. Stiévenard, R.E. Dunin-Borkowski, J. Neugebauer, and P. Ebert, Appl. Phys. Lett. **103**, 152101 (2013).

O 90.8 Thu 12:15 MA 042

Observation of a remarkable reduction of correlation effects in BaCr2As2 by ARPES — •Jayita Nayak[1], Kai Filsinger[1], Gerhard H. Fecher[1], Stanislav Chadov[1], Jan Minár[2], Emile D. L. Rienks[3,4], Bernd Buchner[3,4], Jorg Fink[1,3], and Claudia Felser[1] — [1]Max Planck Institute CPFS, Dresden, Germany — [2]University of West Bohemia,Pilsen, Czech Republic — [3]Institute for Solid State Physics, Leibniz Institute for Solid State and Materials Research Dresden, D- 01171 Dresden, Germany — [4]Institute for Solid State Physics, Leibniz Institute for Solid State and Materials Research Dresden, D- 01171 Dresden, Germany

The superconducting phase in iron-based high-Tc superconductors (FeSC) neighbors a magnetically ordered one in the phase diagram. This proximity hints at the importance of electron correlation effects in these materials. Hunds exchange interaction has been suggested to be the dominant correlation effect in FeSCs because of their multiband nature. Correlation should be strongest for materials closest to a half filled 3d electron shell (Mn compounds, hole-doped FeSCs) and decrease for systems with both higher (electron-doped FeSCs) and lower (Cr-pnictides) 3d counts. Here we find that the strength of correlation effects in nonsuperconducting antiferromagnetic BaCr2As2 is strongly reduced. We have used angle-resolved photoemission spectroscopy (ARPES) and first-principles calculations for this investigation.

O 90.9 Thu 12:30 MA 042

The XPS limit within the one-step model of photoemission: an application to Ag(100) — •Laurent Nicolaï[1], Vladimir Strocov[3], Juraj Krempaský[3], Hubert Ebert[2], Jürgen Braun[2], Federico Bisti[3], and Ján Minár[1] — [1]Univiversity of West Bohemia, Plzeň, Czech Republic — [2]Ludwig-Maximilians-Universität Munich, Germany — [3]Paul Scherrer Institut, Villigen, Suisse

Angle-Resolved Photoemission Spectroscopy (ARPES) is the method of choice for characterising the electronic structure of a given crystalline material. Within the Ultra-Violet (UV) regime, theory can nicely reproduce experimental spectra using the k-conserving dipole selection rules within the one-step model of photoemission [1,2]. Yet, this model is no longer sufficient when dealing with the soft/hard X-ray or high temperature regimes: the XPS-limit. For this case, one has phonon-assisted electronic transitions such that the dipole selection rules cannot describe by themselves the experimentally obtained spectra [3]. Here we use the so-called alloy analogy model in order to quantify the importance of non-dipole transitions. This rather new model is here tested by comparison to new experimental data obtained for the Ag(100) sytem. [1] J. Braun, Rep. Prog. Phys. **59**, 1267-1338 (1996), [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. **74**, 096501 (2011), [3] J. Braun et al., Phys. Rev. B **88**, 205409 (2013)

O 90.10 Thu 12:45 MA 042

The 3D electronic structure of Os(0001) and Re(0001) probed by angle- and spin-resolved soft x-ray photoemission — •Christian Mende[1], Jürgen Braun[1], Jan Minár[2], Hans-Joachim Elmers[3], Gerd Schönhense[3], and Hubert Ebert[1] — [1]Dept. Chemie, LMU München, Germany — [2]NTRC, University of West Bohemia, Plzen, Czech Republic — [3]Institut für Physik, JGU Mainz, Germany

In this contribution we discuss the impact of the spin-orbit coupling on the 3D electronic structure of hcp Os(0001) and Re(0001) as reflected by angle- and spin-resolved soft x-ray photoemission. The spectroscopical analysis has been performed within the framework of the fully relativistic version of the one-step model of photoemission in its spin-density matrix formulation [1]. For this purpose the underlying electronic structure is calculated self-consistently for a semi-infinite half-space configuration using the so called tight-binding (TB) mode of the KKR (Korringa-Kohn-Rostoker) method [2]. To guarantee for a quantitative description of the surface-sensitive spectral features special attention is paid to the image-potential behavior of the surface barrier, which is included as an additional layer in the photoemission formalism. The results that give clear evidence for a pronounced impact of spin-orbit coupling will be discussed in detail in comparison with recent experimental work.

[1] J. Braun et al., New Journal of Physics **16**, 015005 (2014).

[2] H. Ebert et al., The Munich SPR-KKR package, version 7.7.0, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2017).

O 91: 2D materials beyond graphene: TMDCs, silicene and relatives III

Time: Thursday 10:30–13:00 Location: MA 043

O 91.1 Thu 10:30 MA 043

Structure and Electronic Properties of Intrinsic Defects in Single Layer Molybdenum Disulfide on Au(111) — •Christian Lotze, Nils Krane, Asieh Yousofnejad, Gael Reecht, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Germany

Transition metal dichalcogenides (TMDCs) are two-dimensional materials with a natural band gap, making them interesting as sensors, solar cells or LEDs. Single layer molybdenum disulfide (MoS$_2$) 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 combined scanning tunneling/atomic force microscopy (STM/AFM) at low temperatures, we observe different kinds of defects. Particularly prominent are defects, which appear in sizes of several nanometers. NC-AFM reveals an atomically intact surface layer, suggesting that the origin of the defect is located at the gold interface. At these sites, the band gap of MoS$_2$ is significantly modified, pointing towards quasi-freestanding MoS$_2$ on a metal substrate [3]. Moreover, we identify single point defects like Mo and S vacancies by STM/AFM and tunneling spectroscopy. The latter two exhibit localized in-gap defect states, which agree well with simulations from density functional theory [4].

[1] Mak *et al.*, PRL **105**, (2010) 136805; [2] Sorensen, *et al.*, ACS Nano **8**, (2014) 6788; [3] Krane, *et al.*, Nano Lett. **16**, (2016) 5163; [4] González, *al.*, Nanotechnology, **27** (2016), 105702

O 91.2 Thu 10:45 MA 043

Structural vs Electronic Effects in the Moiré Pattern of MoS$_2$ on Au(111) — •Daniela Dombrowski[1,2], Caio Silva[1], Nicolae Atodiresei[3], Wouter Jolie[1,2], Ferdinand Farwick zum Hagen[2], Pardeep Thakur[4], Vasile Caciuc[3], Thomas Michely[2], Stefan Blügel[3], Tien-Lin Lee[4], and Carsten Busse[1,2,5] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [4]Diamond Light Source, United Kingdom — [5]Department Physik, Universität Siegen, Germany

Scanning tunneling microscopy (STM) measurements of molybdenum disulfide (MoS$_2$) grown on Au(111) show a strong corrugation of the moiré pattern, arising from the lattice mismatch between the MoS$_2$ layer and the underlying gold substrate. However, STM measurements do not give a pure structural information, since the tip follows the contour of a constant density of states. We combine low temperature scanning tunneling spectroscopy (STS) and x-ray standing wave (XSW) measurements with density functional theory calculations (DFT) to separate structural and electronic contributions to the moiré modulation. Our XSW measurements indicate that MoS$_2$ on gold is nearly flat in agreement with DFT calculations, giving a corrugation of 0.3 Å. In STS measurements we observe a significant shift of the valence band edge, following the moiré periodicity. This suggests that the observed corrugation in STM has mainly an electronic nature.

O 91.3 Thu 11:00 MA 043

Synthesis and properties of single-layer VS$_2$ on Au (111) — •Raluca-Maria Stan[1], Fabian Arnold[1], Charlotte Sanders[1], Albert Bruix[1], Sanjoy Mahatha[1], Henriette Lund[1], Maciej Denzik[1], Davide Curcio[1], Harsh Bana[2], Elisabetta Travaglia[2], Luca Bignardi[3], Paolo Lacovig[3], Daniel Lizzit[3], Marco Bianchi[1], Jill Miwa[1], Martin Bremholm[4], Silvano Lizzit[3], and Philip Hofmann[1] — [1]Dep. of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Aarhus, Denmark. — [2]Dep. of Physics, University of Trieste, Trieste, Italy. — [3]Elettra - Sincrotrone Trieste S.C.p.A., Trieste, Italy. — [4]Dep. of Chemistry, University of Aarhus, Aarhus, Denmark.

The single-layer (SL) transitional metal dichalcogenide vanadium disulfide (VS$_2$) has attracted interest due to predicted intrinsic ferromagnetism that could be exploited in future spintronic applications and data storage devices. For the first time, SL VS$_2$ of the 1T variety has been synthesized on Au (111). The SL has metallic character and a strong preference to form triangular islands with a moiré superstructure and a well-defined orientation with respect to the substrate. Annealing to temperatures higher than 450 °C, two phase transitions are observed: one phase exhibits a distorted hexagonal unit cell while the other one has a rectangular unit cell characterized by a sulfur deficiency. The unexpected latter phase is reached upon annealing in ultra-high vacuum to temperatures higher than 550 °C. The transition between these phases is reversible upon annealing at lower temperatures in high H$_2$S pressure.

O 91.4 Thu 11:15 MA 043

Structural and electronic characterization of sulfur depleted monolayer VS2 synthesized on Au(111) — •Umut Kamber[1], Fabian Arnold[2], Brian Kiraly[1], Raluca-Maria Stan[2], Arlette Sohanfo Ngankeu[2], Marco Bianchi[2], Jill Miwa[2], Charlotte Sanders[2], Philip Hofmann[2], and Alexander Ako Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark

Studies on bulk transition metal dichalcogenides (TMDCs) show a variety of electronic properties based on the specific combination of metal and chalcogen elements. Since it is possible to exfoliate or synthesize stable 2D versions of many TMDCs, they have attracted great attention for the opportunity to study reduced dimensionality in a variety of electronic systems. VS2 is of particular interest, as it has not yet been synthesized in monolayer form, and its magnetic ground state is unclear. Here, we present an investigation with low temperature scanning tunneling microscopy/spectroscopy (STM/STS) on the structural and electronic properties of sulfur-depleted single layer VS2 on Au(111). Upon annealing as grown 1T monolayer VS2, there is a structural phase transition to a sulfur depleted phase of VS2, which exhibits reconstructed chain-like structures. Our results shed light on the atomic structure of single layer VS2 as well as reveal a complex Fermi surface of striped phase. STS mapping at low temperature indicates the emergence of non-dispersive electronic ordering close to the Fermi level.

O 91.5 Thu 11:30 MA 043

Bismuth-intercalated WS$_2$ on Ag(111): a nearly free-standing single-layer TMDC — •Maciej Dendzik[1,2], Sanjoy Mahatha[2], Charlotte Sanders[2], Matteo Michiardi[2,3], Marco Bianchi[2], Jill Miwa[2], and Philip Hofmann[2] — [1]Department of Physical Chemistry, Fritz-Haber-Institut of the Max Planck Society, Faradayweg 4-6, Berlin 14915, Germany — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, BC V6T 1Z1, Canada

Recent developments in the field of two-dimensional transition metal dichalcogenides (TMDCs) have shown that the substrate can have a profound effect on the electronic band structure of these materials [1-3]. For example, a semiconducting single-layer (SL) WS$_2$ was found to be metallic when grown on Ag(111) [4]. Here we demonstrate that bismuth intercalation can be used to effectively decouple SL WS$_2$ from the substrate. Angle-resolved photoemission spectroscopy (ARPES) measurements indicate a nearly free-standing character of WS$_2$ after intercalation. Low-energy electron diffraction (LEED) and scanning-tunneling microscopy (STM) results shed further light on the crystal structure of the investigated WS$_2$-Bi-Ag complex.

[1] J. A. Miwa *et al.*, Phys. Rev. Lett., **114**, 046802, 2015.
[2] M. Dendzik *et al.*, Phys. Rev. B, **92**, 245442, 2015.
[3] C. E. Sanders *et al.*, Phys. Rev. B, **94**, 081404 (R), 2016.
[4] M. Dendzik *et al.*, Phys. Rev. B, *in press.*

O 91.6 Thu 11:45 MA 043

***In situ* growth and characterization of single-layer molybdenum disulfide on Au(111)** — •Moritz Ewert[1,2], Lars Buss[1], Jens Falta[1,2], and Jan Ingo Flege[1,2] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]MAPEX Center for Materials and Processes, Bremen, Germany

Single-layer (SL) transition metal dichalcogenides are in today's research focus due to their electronic similarity to graphene as well as owing to their catalytic properties, e. g., in hydrodesulfurization processes.

We have investigated the growth of SL molybdenum disulfide (MoS_2) on Au(111) by Mo metal deposition in dimethyldisulfide background using low-energy electron microscopy (LEEM) and microdiffraction (μLEED). In situ investigations at different elevated temperatures reveal that triangular MoS_2 islands nucleate and continue to grow in a dendritic mode, extending over several square μm in size. The local structure of the islands was elucidated by analyzing the specular electron reflectivity depending on electron energy measurements (IV-LEEM), confirming the sole existence of SL structures. This finding is corroborated by μLEED, which demonstrates the formation of micron-sized MoS_2 SL domains. Furthermore, closer investigation of the mesoscale structure in dark-field LEEM shows that the triangular-shaped structures can be found in two distinct orientations, whose relative abundance has been found to depend on temperature.

O 91.7 Thu 12:00 MA 043

Spin structure of the K valleys in single-layer WS_2 on Au(111) — •Philipp Eickholt[1], Albert Bruix[2], Marcel Holtmann[1], Charlotte Sanders[3], Marko Bianchi[3], Philip Hofmann[3], and Markus Donath[1] — [1]Westfälische-Wilhelms-Universität Münster, Germany — [2]TU München, Germany — [3]Aarhus University, Denmark

In the field of 2D materials, single-layer transition metal dichalcogenides, especially MoS_2, WS_2, $MoSe_2$, and WSe_2, play an important role. Due to their exceptional optical and electronic properties, they are promising materials for optoelectronical applications. The key to understand the material properties is a profound knowledge of the electronic structure. The occupied electronic structure was investigated in a number of studies, yet without spin resolution. In addition, no experimental information concerning band dispersion and spin structure of the conduction bands is available so far.

We present measurements of a combined spin- and angle-resolved direct and inverse photoemission experiment, performed within the same apparatus [1,2]. Our results unravel the spin-dependent energies of the valence- and conduction bands at the K and K' valleys, which are decisive for the optoelectronic properties of the materials.

[1] M. Budke *et al.*, Rev. Sci. Instrum. 78, 113109 (2007)

[2] S.D. Stolwijk *et al.*, Rev. Sci. Instrum. 85, 013306 (2014)

O 91.8 Thu 12:15 MA 043

Pseudodoping of single-layer TaS_2 on Au(111) — Bin Shao[1], •Andreas Eich[2], Charlotte Sanders[3], Arlette Sohanfo Ngankeu[3], Marco Bianchi[3], Philip Hofmann[3], Alexander Ako Khajetoorians[2], and Tim Oliver Wehling[1] — [1]Institut fuer Theoretische Physik (ITP), and Bremen Center for Computational Materials Science (BCCMS), Universitaet Bremen, Germany — [2]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [3]Department of Physics and Astronomy, Interdisciplinary Science Center (iNANO), Aarhus University, Denmark

We demonstrate how weak hybridization of a monolayer of TaS_2 grown on Au(111) can lead to an apparent heavy doping. Combining *ab-initio* calculations and a generic model, we show that strong reshaping of Fermi surfaces and changes in Fermi volumes can arise without actual charge transfer. This mechanism, which we refer to as pseudodoping, explains particular features in the DOS found in the experimental data which are not present in the calculated freestanding case. Moreover, we discuss experimentally observed defects in the TaS_2 monolayer, and illustrate how the changes in hybridization change the experimentally observed features on the LDOS. Finally, we illustrate theoretically that this is a generic effect for metallic 2D materials which are either weakly absorbed to metallic substrates or embedded in vertical heterostructures.

O 91.9 Thu 12:30 MA 043

Synthesis of large area and high-quality MoS_2 monolayers with single domain orientation on Au(111) — Harsh Bana[1], Elisabetta Travaglia[1], •Luca Bignardi[2], Paolo Lacovig[2], Charlotte E. Sanders[3], Maciej Dendzik[3], Matteo Michiardi[3], Marco Bianchi[3], Daniel Lizzit[2], Francesco Presel[1], Dario De Angelis[1], Nicoleta Apostol[4], Pranab Kumar Das[5,6], Jun Fujii[6], Ivana Vobornik[6], Rosanna Larciprete[7], Alessandro Baraldi[1,2,6], Philip Hofmann[3], and Silvano Lizzit[2] — [1]University of Trieste, Trieste, Italy — [2]Elettra Sincrotrone Trieste, Trieste, Italy — [3]University of Aarhus, Aarhus, Denmark — [4]Nat. Inst. Material Physics, Magurele, Romania — [5]Int. Center Theor. Physics, Trieste, Italy — [6]Ist. Officina Materiali-CNR, Trieste, Italy — [7]Ist. Sistemi Complessi-CNR, Rome, Italy

The implementation of MoS_2-based devices exploiting the valley-spin degree of freedom relies on the presence of singly-oriented crystalline domains in the layer, which is not secured by current growth methods. We present a protocol for the synthesis through physical vapor deposition of single-layer (SL) MoS_2 with a single orientation on Au(111) and we characterize the layer with a combination of surface science techniques. Photoelectron diffraction (XPD) proved the single orientation character of the layer, while STM and angular resolved photoemission (ARPES) confirmed the high structural quality. The single domain orientation allowed the measurement, through spin-resolved ARPES, of the complete spin polarization with spin reversal of the states near K and -K points.

O 91.10 Thu 12:45 MA 043

Photocatalytic properties of MoS2 membranes — •Matthias Golibrzuch[1], Elmar Mitterreiter[1,2], Eric Parzinger[1,2], Max Stelzer[3], Franz Kreupl[3], Joel Ager III[4,5], Alexander Holleitner[1,2], and Ursula Wurstbauer[1,2] — [1]Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Am Coulombwall 4a — [3]Department of Hybrid Electronic Systems, Technische Universität München, 80333 München, Germany — [4]Electronic Materials Program, Materials Sciences Division, Lawrence Berkeley National Laboratory — [5]Deptartment of Materials Science and Engineering, University of California, Berkeley, CA 94720

MoS2 is a fascinating two-dimensional van der Waals material with outstanding electronic, optical and catalytic properties. Its high optical absorption up to 15% in the visible range for monolayers together with catalytic activity and photocatalytic stability makes single-layer MoS2 a very promising material for sunlight driven photocatalytic applications such as photocatalytic hydrogen evolution (HER).

We demonstrate the photocatalytic activity regarding HER of exfoliated single- and few-layer MoS2 immersed in an acid electrolyte by cyclic voltammetry. We observe an increased catalytic activity of MoS2 with decreasing number of layers. In particular, monolayers exhibit high current densities, low onset potentials and high turnover frequencies. Edge sites and defects show higher activities than the basal plane. We furthermore demonstrate that HER activity is increased by illumination in the visible range.

O 92: Nanostructures at surfaces: Dots, particles, clusters I

Time: Thursday 10:30–13:00 Location: MA 141

Invited Talk O 92.1 Thu 10:30 MA 141

0-D and 1-D heterostructure mediated material properties of 2-D Transition Metal Dichalcogenides — •Alexander Weber-Bargioni — Lawrence Berkeley National Laboratory, Berkeley, Ca, USA

In this presentation we show how individual atomic defects and linear mirror twin boundaries in 2-D MoSe2, identified with super resolution atomic force microscopy, alter the electronic wave function, imaged via Scanning Tunneling Spectroscopic mapping, leading along mirror twin boundaries to charge density waves and solitons.

Hierarchically ordered defects or adsorbents in two dimensional transition metal dichalcogenides (TMDs - MoS2, WS2, MoSe2, etc*) modify the local electronic states in terms of energy and geometry of the electronic wave functions at length scales of individual wave functions, inducing novel functionality. Due to their 2-D nature, 2-D TMDs are an excellent model system to directly access, visualize and determine the effects of defect mediated electronic wave function tuning using high resolution AFM and differential conductance mapping.

We show the rich, localized electronic structure of individual vacancies and atomic replacements creating 0-D heterostructure, and how 1-D defects can undergo quantum phase transitions creating charge density waves and solitons.

O 92.2 Thu 11:00 MA 141

Thin films of hydrogen-terminated silicon nanoparticles on functionalized surfaces — •Domenikos Chryssikos[1], Markus Wiesinger[1], Martin Stutzmann[1], Anna Cattani-Scholz[1], and Rui N. Pereira[1,2] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching bei München, Germany — [2]Department of Physics and Institute for Nanostructures, Nanomodelling and Nanofabrication, University of Aveiro, 3810-193 Aveiro, Portugal

Electronic devices incorporating thin films of solution-processed crystalline nanoparticles (NPs) of semiconductor materials have been studied intensively in recent years as an alternative to bulk materials. Silicon is advantageous for use in the form of NPs, thanks to its abundance and non-toxicity. However, thin films of silicon NPs (SiNPs) with H-termination, required for efficient charge transport, are difficult to achieve due to NP agglomeration in solution. In this work, we explore the assembling of thin films of H-terminated SiNPs bound to silicon dioxide surfaces functionalized with a monolayer of decyldiphosphonic acid molecules. We expect this method to provide a stable and patternable immobilization of very thin layers of SiNPs. Deposition of SiNPs can be realized via substrate immersion in SiNP colloid, followed by annealing at 140°C. By comparison with control samples, our results indicate the requirement of substrate functionalization and annealing for a stable, sonication-resistant attachment of SiNPs to the substrates. Further, the electrical properties of the obtained SiNP networks are studied by means of bottom-gate field-effect transistors.

O 92.3 Thu 11:15 MA 141

Towards atomic-scale switches based on self-assembled surface magic clusters — •Martin Franz[1], Jan Grosse[1], Tim Amrhein[1], Chiara Panosetti[2], Karsten Reuter[2], and Mario Dähne[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Department Chemie, Technische Universität München, D-85748 Garching, Germany

Atomic-scale switches represent the ultimate level of device miniaturization. Here, we present the first example of such a switch based on self-assembled magic clusters on surfaces.

Using scanning tunneling microscopy and density functional theory, we find that so-called centered rare earth silicide clusters forming self-assembled on the Si(111)7×7 surface [1,2] show a bistable switching between two mirror symmetric configurations. Thereby, a rather high energy barrier of 1.3 eV between the configurations suppresses a thermally induced flipping even at room temperature. In the presence of a close STM tip, however, the clusters start flipping between the two configurations indicating a tip-induced lowering of the barrier height, leading to the possibility to intentionally switch the clusters from one configuration to the other and back.

This work was supported by the DFG, FOR 1282, projects D and H.

[1] M. Franz, S. Appelfeller, M. Rychetsky, and M. Dähne, Surf. Sci **609**, 215 (2013).
[2] M. Franz, J. Große, R. Kohlhaas, M. Dähne, and Surf. Sci. **637-638**, 149 (2015).

O 92.4 Thu 11:30 MA 141

Directional and Angular Locking in the Stick-Slip Motion of Au Islands on a Natural MoS2 Crystal Surface — •Felix Trillitzsch — Otto-Schott-Institut für Materialforschung, Friedrich-Schiller-Universität Jena

Atomic force microscopy (AFM) nanomanipulation experiments have been performed on triangular Au islands (with typical linear size of 25-80 nm) previously grown on a MoS2 surface in ultra-high vacuum (UHV) conditions. In ambient conditions the islands are found to move along well-defined preferential directions, independently of the angle of attack of the AFM probe. Molecular dynamics simulations prove that these directions corresponds to the principal crystallographic orientations of the substrate. Additionally, the islands almost never rotate during manipulation, except for a slight wobbling motion (with an estimated angular oscillation amplitude well below 1°). This is very different from AFM-based manipulation experiments with lattice-mismatched contact interfaces, where the direction of motion is determined by the geometry of the problem and roto-translational motion is observed. Apart from shedding light on the fundamental mechanisms of friction our results may find important applications in the controlled positioning of metal islands as electrodes for molecular electronics.

O 92.5 Thu 11:45 MA 141

Investigation of core-shell nanoparticles using scanning transmission x-ray microscopy (STXM) — •Anja Hermanns[1], Sufal Swaraj[2], Thomas Heinrich[1], Caterina Minelli[3], Katia Sparnacci[4], and Wolfgang Unger[1] — [1]Bundesanstalt für Materialforschung und -prüfung, 12203 Berlin, Germany — [2]Synchrotron SOLEIL, 91190 Saint-Aubin, France — [3]National Physical Laboratory, Teddington TW11 0LW, United Kingdom — [4]Università del Piemonte Orientale, 15121 Alessandria, Italy

Products containing nanoparticles encounter us in almost all areas of our daily life. In most cases the particles exhibit a core-shell morphology either voluntarily or involuntarily. The properties of the shell determine the interaction of the particles with their environment and, thus, reliable control over these properties means reliable control over the performance of the particles. Beside its chemical composition, the thickness of the shell is a parameter of utmost importance. A scanning transmission x-ray microscopy (STXM) based methodology is presented for determining the dimensions (shell thickness, core and total diameter) of core-shell nanoparticles which exhibit a strong x-ray absorption contrast and a well-defined interface between core and shell material. The authors acknowledge support from the European Metrology Programme for Innovation and Research (EMPIR) as part of the InNanoPart 14IND12 project. The EMPIR initiative is cofunded by the European Unions Horizon 2020 research and innovation programme and by the EMPIR participating states.

O 92.6 Thu 12:00 MA 141

Tailoring gold cluster growth during sputter deposition on polymer surfaces via pressure and bias voltage. — •Matthias Schwartzkopf[1], Oleksandr Polonskyi[2], Alexander Hinz[2], Thomas Strunskus[2], Franziska C. Löhrer[3], Volker Körstgens[3], Franz Faupel[2], Peter Müller-Buschbaum[3], and Stephan V. Roth[1,4] — [1]DESY, 22607 Hamburg — [2]CAU, 24143 Kiel — [3]TUM, 85748 Garching — [4]KTH, 10044 Stockholm

The utilization of sputter deposition stands out as a versatile routine method in industry and science to precisely adjust properties of metal coatings depending on the application requested. In order to obtain full control over the nanostructural evolution at the metal-polymer interface, we employed time-resolved surface sensitive X-ray scattering (GISAXS) during sputter deposition of gold on thin polystyrene films [1,2]. We correlate the evolution of the metallic layer morphology with changes in the key scattering features. We identify the impact of atomic deposition rate, noble gas pressure and bias voltage on the growth regimes. Whereas the deposition rates effects mainly the nucleation and cluster percolation, the gas pressure and bias voltage influence the degree of order in the cluster assembly. [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015); [2] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017).

O 92.7 Thu 12:15 MA 141

In-situ investigation of metallic nanoparticle growth in a gas aggregation source — •Oleksandr Polonskyi, Alexander Vahl, Jonas Drewes, Alexander Hinz, Thomas Strunskus, and Franz Faupel — Chair for Multicomponent Materials, Faculty of Engineering, Kiel University, Germany

Metallic nanoparticles play an important role in the growing field of nanotechnology due to the unique properties associated with their small dimensions. Recently, so-called gas aggregation nanoparticle sources (GAS) (Haberland type, based on magnetron sputtering) have become very attractive for nanoparticle generation and they provide the ability to deposit various types of NPs with good control over size and size distribution. However, the processes inside the GAS are not fully understood yet, even though the GAS has often been used for generation of metallic clusters and nanoparticles. We report on the investigation of the initial stages of Ag nanoparticle growth in a gas phase by broadband transmission UV-Vis spectroscopy. We demonstrate that due to their strong particle plasmon resonance, small clusters and nanoparticles can be monitored by UV-Vis spectroscopy in-situ during growth and transport. We found that small clusters are already generated in the region close to the magnetron target surface and generally do not change their size much during transport through the gas aggregation chamber. Our measurements indicate that a high concentration of nanoparticles is located near the magnetron and results in strong coupling between neighboring particle plasmon resonances.

O 92.8 Thu 12:30 MA 141

Winkelaufgelöste Photoelektronenspektroskopie an massenselektierten Silberclustern — •Norman Iwe, Franklin Martinez, Josef Tiggesbäumker und Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, Albert-Einstein-Str. 23-24, 18059 Rostock, Deutschland

Die Photoelektronenspektroskopie ermöglicht die Untersuchung der elektronischen Struktur atomarer Cluster. Zum einen lassen sich aus der Energie der mittels Photoeffekt emittierten Elektronen Rückschlüsse auf deren Bindungsenergien im Cluster ziehen. Zum anderen enthält die Emissionsrichtung der Elektronen Informationen über den Drehimpulscharakter ihres ursprünglichen Bindungszustands.

In diesem Beitrag werden winkelaufgelöste Photoelektronenspektren von massenselektierten Silberclusteranionen vorgestellt und diskutiert. Für das Silber-Trimer experimentell bestimmte Anisotropie-Parameter werden mit Vorhersagen des Jellium-Modells verglichen.

O 92.9 Thu 12:45 MA 141

Single-molecule fluorescence excited by a scanning tunnelling microscope — •Jörg Kröger[1,2], Benjamin Doppagne[2], and Guillaume Schull[2] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Institut de Physique et Chimie des Matériaux de Strasbourg, F-67034 Strasbourg, France

Ultrathin NaCl films on Ag(111) were used to efficiently decouple the organic electron donor molecule tetraphenyldibenzoperiflanthene ($C_{64}H_{36}$, DBP) from the metal support and to probe the genuine molecular luminescence. Injecting charge from the tip of a low-temperature scanning tunnelling microscope into DBP leads to photon emission with different quantum yields across the molecule reflecting the presence of a single transition dipole moment. Vibrational progression and hot electroluminescence may be inferred from the photon spectra. By placing the tip in the lateral nanometre vicinity of the molecule light emission is remotely controlled. The spectral line shape of the excited $S_1 \longrightarrow S_0$ transition exhibits a Fano profile whose asymmetry varies with the tip-molecule distance. These data reflect the subtle interplay between the injected charge, the molecular exciton and the plasmonic environment. Financial support by the Deutsche Forschungsgemeinschaft through Grant No. KR 2912/12-1 is acknowledged.

O 93: Focus Session: Structural Dynamics in Nanoscale Materials, Probed by Ultrafast Electron Pulses I

Time: Thursday 10:30–13:00 Location: HE 101

Invited Talk O 93.1 Thu 10:30 HE 101

Ultrafast Electron Diffuse Scattering: Mapping Momentum Dependent Electron-Phonon Coupling and Nonequilibrium Phonon Dynamics in 2D Materials — •Bradley Siwick[1,2], Martin Otto[1], Laurent Rene de Cotret[1], Mark Stern[1], and Mark Sutton[1] — [1]McGill University, Department of Physics, Center for the Physics of Materials, Montreal, Canada — [2]McGill University, Department of Chemistry, Montreal, Canada

The nature of the couplings within and between lattice and charge degrees of freedom is central to condensed matter and materials physics. These interactions are determining to phenomena as diverse as superconductivity, charge density waves and carrier mobility in semiconductors and metals. Despite their fundamental role, detailed momentum-dependent information on the strength of electron-phonon and phonon-phonon coupling across the entire Brillouin zone has proved elusive. This talk will describe a new technique, ultrafast electron diffuse scattering (UEDS), that can provide such information. Specific applications of UEDS to 2D materials will be presented.

Invited Talk O 93.2 Thu 11:00 HE 101

Beyond Debye-Waller Effects in Ultrafast Electron Diffraction — •Xijie Wang — SLAC National accelerator Labotorary, Menlo Park, CA 94025, USA

Transient Debye Waller-effects has been used extensively for studying energy relaxation and lattice heating in laser excited materials in time-resolved X-ray or electron diffraction. In this talk, I will discuss the latest developments in MeV ultrafast electron diffraction and its applications for structure dynamics. Taking advantage negligible multiple scattering of MeV electrons in the materials, we successfully extended the transient Debye*Waller-effects to study the energy relaxation and transport in nano-scale heterostructure, ripples and energy relaxation in 2-D materials and phonon-phonon coupling in diffuse scattering. I will also discuss multi-modal studies of quantum materials at SLAC MeV UED.

O 93.3 Thu 11:30 HE 101

Ultrafast nanotectonics with nanocrystalline graphene — Silvio Morgenstern, •Arne Senftleben, Marlene Adrian, Christian Gerbig, and Thomas Baumert — Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel

Nanocrystalline graphene consists of nanometer-sized plates with a perfect graphene structure, which are coupled to each other via lattice defects containing sp^3 hybridized carbon atoms. When heated, the plates expand and the sp^3 hybrids act as a hinge. The result is a nano-scale movement that recalls the formation of wrinkled mountains. Here we report on expansion time scales in the 100 fs regime followed by out of plane dynamics on the sub ps time scale on a free standing nanocrystalline graphene sheets with the help of our high resolution ultrafast electron diffraction apparatus.

O 93.4 Thu 11:45 HE 101

Molecular dynamics simulations of a femtosecond laser excitation in antimony — •Bernd Bauerhenne[1,2], Felipe Valencia[3], and Martin E. Garcia[1,2] — [1]Theoretische Physik - Universität Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany — [2]Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), Heinrich-Plett-Strasse 40, D-34132 Kassel, Germany — [3]Physics Department, Universidad Nacional de Colombia, Edificio 404, Ciudad Universitaria, Bogota, Colombia

The goal of this work is to accurately simulate laser induced ultrafast, nonthermal solid-to-solid and solid-to-liquid phase transitions in Sb. In particular we are interested in elucidate the dynamics of the ultrafast transition from the A7 to the simple cubic structure in Sb, and also to investigate how fast nonthermal melting of Sb can occur for extremely high laser fluences. For this purpose, we run ab-initio molecular dynamic simulations of laser excited antimony in thin-film geometry (containing around 400 atoms) using our in house density functional theory code CHIVES. Based on these simulations and in order to allow for a closer comparison with experiments, we developed an analytical interatomic potential describing laser excited Sb. In addition, we calculated the laser-fluence dependent electron-phonon coupling constant in Sb from ab-initio calculations. Using our potential and including incoherent electron-phonon scattering, we simulated the intense femtosecond laser excitation of antimony on large supercells.

O 93.5 Thu 12:00 HE 101

Electron-Phonon coupling in thin Pb films on Si(111) from the lattice's perspective — •Tobias Witte, Tim Frigge, Bernd Hafke, Boris Krenzer, and Michael Horn-von Hoegen — Universität Duisburg-Essen, 47048 Duisburg, Germany

Employing time resolved reflection high energy electron diffraction (tr-RHEED) the non-equilibrium dynamics of the phonon system after optical excitation of ultrathin Pb films and islands on Si(111) has been investigated. The sample is pumped by fs-IR-laserpulses, while the transient response is probed by 30 keV electron pulses. Surface sensitivity is achieved through gracing incidence of the high energy electrons. fs-laserpulses cause impulsive excitation of the electron system of the Pb films and islands, respectively. The hot electron system thermalizes and heats the lattice system by electron-phonon coupling. The thermal motion of the (surface-) atoms is observed through the transient Debye-Waller effect. As Pb is known to exhibit strong electron-phonon coupling in the bulk the time constant for the energy transfer to the lattice system is - in the framework of the two temperature model - expected to be in the sub-ps regime. In contrast, a rather slow time constant of $\tau = 3.2$ ps was observed at the surface. Moreover, incoherent lattice excitation of the islands occurs even slower at a time constant of $\tau = 4.6$ ps. These results demonstrate how low-dimensionality and quantum-size effects reduce the energy flow mediated by electron-phonon coupling.

O 93.6 Thu 12:15 HE 101

Efficient simulation scheme for propagation of energetic electrons in solids. — •Beata Ziaja-Motyka — CFEL, DESY Hamburg, Germany — INP PAS Krakow, Poland

Intense X-rays pulses, while irradiating solids, excite energetic photoelectrons. In case of inner-shell photoionization, frequent with hard X-rays, the core holes left after the photoionization relax predominantly through Auger decays, accompanied by emission of further electrons. Both photo- and Auger electrons ionize the sample through impact ionization, releasing further electrons. Those collisional processes then trigger secondary electron cascades which significantly contribute to the progressing damage of the sample.

Here we report on a dedicated Monte Carlo code able to accurately follow spatial and temporal evolution of electron cascades in solids under low-fluence X-ray pulse irradiation (implying moderate density of excited electrons). This computationally efficient scheme uses an 'independent cascade' approximation. We discuss an extension of the code to simulate propagation of excited electrons in a bulk material under intense X-ray irradiation - preserving its high computational efficiency. If successful, the tool can be applied for radiation damage studies of X-ray diffraction as well as of electron diffraction, as relaxation of a material excited by a highly energetic electron projectile is similar to that after an X-ray excitation.

O 93.7 Thu 12:30 HE 101

Direct Observation of Reaction Dynamics by Femtosecond Electron Diffraction — •Henrike Müller-Werkmeister[1,2], Yifeng Jiang[1], Lai Chung Liu[3], and R. J. Dwayne Miller[1,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, 22607 Hamburg, Germany — [2]Institute of Chemistry, Physical Chemistry, University of Potsdam, 14476 Potsdam, Germany — [3]Departments of Chemistry and Physics, University of Toronto, Toronto, M5S 3H6, Canada

Femtosecond electron diffraction (FED) is a sensitive tool to directly study molecular dynamics in structural detail. We have studied the photoinduced spin crossover (SCO) in the coordination compound [FeII(PM-AzA)2](NCS)2 (or AZA). The unique capability of FED allows us to directly probe atomic motions and to track ultrafast structural changes within the crystal lattice of AZA. The data and refinement calculations indicate the global structural reorganization within 2.3 ps, as the metal-to-ligand bond distribution narrows during intramolecular vibrational energy redistribution (IVR), driving the molecular rearrangement. Three independent dynamical groups are identified to model the structural dynamics upon photoinduced SCO.

Y. Jiang, L. Liu, H. M. Müller-Werkmeister, C. Lu, D. Zhang, R. L. Field, A. Sarracini, G. Moriena, E. Collet, and R. J. D. Miller, Angew. Chemie 129, 7236 (2017).

O 93.8 Thu 12:45 HE 101

Ultrafast pathways of the photo-induced insulator-metal transition in an organic molecular crystal — Bart Smit[1], Florian Hüwe[2], Nancy Payne[1], Olufemi Olaoye[1], Irene Bauer[3], Jens Pflaum[2], Markus Schwoerer[3], and •Heinrich Schwoerer[1,4] — [1]Stellenbosch University, South Africa — [2]Universität Würzburg, Deutschland — [3]Universität Bayreuth, Deutschland — [4]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland

Low dimensional molecular metals represent an intriguing class of solid functional organic materials due to their tunable electronic, dielectric, magnetic and structural ground states. We report on the collective atomic motion at the insulator-to-metal Peierls transition of the radical ion salt Cu(Me,Br-DCNQI)2 (DCNQI: Dicyanoquinonediimine), detected by ultrafast electron diffraction. We observe the photo-induced lifting of the insulating phase within 2 ps in the entire crystal volume, which enables high-speed optical sensors of outstanding signal response. We uncover that the phase transition is initiated by specific collective bending mode within the organic molecule, however, only an additional internal pressure relief, manifested by a volume growth of rest groups, allows to optically lock the metallic state for long times. The disclosing of the microscopic pathways to optically drive the structural Peierls transition in Cu(DCNQI)2 points out the tailored response to external stimuli available in this unique class of complex functional materials.

O 94: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Thursday 10:30–12:45 Location: HL 001

O 94.1 Thu 10:30 HL 001

Core-level spectroscopy with the *GW* approximation — •Dorothea Golze and Patrick Rinke — Department of Applied Physics, Aalto University, Espoo, Finland

Inner-shell spectroscopy is an important tool to characterize molecules, liquids and adsorption processes at surfaces. We present a new, accurate method for computing X-ray photoelectron spectra based on the *GW* approximation that overcomes the limitations of density functional theory based approaches. Green's function theory in the *GW* approximation has become the method of choice for addition and removal energies of valence electrons in solids and is now increasingly being applied to molecules. However, *GW* core-level spectroscopy has thus far not received any attention. In most *GW* implementations, the self-energy is computed in the imaginary frequency domain followed by an analytic continuation to the real frequency axis. However, our calculations show that the analytic continuation becomes highly inaccurate for frequencies far away from the Fermi level and is not suitable for the computation of core excitations. Thus, we evaluate the self-energy on the real-frequency axis using the contour deformation (CD) technique.

We implemented CD in combination with a resolution-of-the-identity approximation for the screened Coulomb interaction in the FHI-aims program package. Test calculations reveal that our implementation reproduces Turbomole reference calculations [1] perfectly. Furthermore, we present benchmark studies of small and medium-sized gas-phase molecules and discuss the potential of our method for more complex systems. [1] M. J. van Setten et al. JCTC, 2013, 232

O 94.2 Thu 10:45 HL 001

***GW* and beyond from matrix resolvents** — •Jan Gesenhues[1], Dmitrii Nabok[2], Michael Rohlfing[1], and Claudia Draxl[2] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Theoretische Festkörperphysik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Typically GW calculations make use of either plasmon pole models or numerical integration in order to determine the screened Coulomb interaction W. We demonstrate how to obtain an analytical representation of W with the help of a matrix resolvent and present some standard GW results which have been obtained with the method. The analytical W is a useful starting point for subsequent calculations involving vertex corrections. On the other hand, the matrix resolvent technique itself can be applied upon a BSE-like equation of motion for the polarizability to include vertex corrections.

O 94.3 Thu 11:00 HL 001

Electron-Magnon Scattering in Elementary Ferromagnets from First Principles: Lifetime Broadening and Kinks — 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

We study the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory implemented in the full-potential linearized augmented-plane-wave method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the two-particle (electron-hole) Green function, where single-particle Stoner excitations and collective spin-wave excitations (magnons) are treated on the same footing. We employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. The resulting renormalized electronic band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy, which are strongest in Fe. In the case of Co and Ni, the renormalization gives rise to kinks in the electronic band dispersion at low binding energies, which we attribute to electron scattering with spatially extended spin waves. Furthermore, we find a band anomaly at larger binding energies in iron, which results from a coupling of the quasihole with single-particle excitations that form a peak in the Stoner continuum. This band anomaly has, in fact, been observed in recent photoemission experiments at the same energy and momentum.

O 94.4 Thu 11:15 HL 001

Effects of the Tamm-Dancoff approximation on the optical spectra of organic molecules — •Tobias Lettmann and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

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

It is generally accepted that the TDA is justified for large, extended systems e.g. bulk crystals. However it has been shown that the TDA may no longer hold for some organic semiconductors[1]. In this talk we discuss the effects of the TDA on the resulting optical spectra of organic molecules of different sizes and investigate for which cases the TDA may still be justified.

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

O 94.5 Thu 11:30 HL 001

Ab-initio treatment of non-local electronic correlations with the dynamical vertex approximation — •Anna Galler[1], Patrik Thunström[2], Patrik Gunacker[3], Josef Kaufmann[3], Matthias Pickem[3], Jan M. Tomczak[3], and Karsten Held[3] — [1]Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau, France — [2]Department of Physics and Astronomy, Materials Theory, Uppsala University, 75120 Uppsala, Sweden — [3]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

Recently, approaches such as the dynamical vertex approximation (DΓA) or dual-fermion method have been developed. These diagrammatic approaches are going beyond dynamical mean-field theory (DMFT) by including non-local electronic correlations on all length scales as well as the local DMFT correlations. Here we present our efforts to extend the DΓA methodology to ab-initio materials calculations (AbinitioDΓA). Our approach is a unifying framework which includes both, GW and DMFT-type of diagrams, but also important non-local correlations beyond, e.g. non-local spin fluctuations. In our multi-band implementation we are using a worm sampling technique within continuous-time quantum Monte Carlo in the hybridization expansion to obtain the DMFT vertex, from which we construct the reducible vertex function in a ladder approximation. As a first application we show results for transition metal oxides. Support by the ERC project AbinitioDGA (306447) is acknowledged.

References: [1] A. Galler, P. Thunström, P. Gunacker, Jan M. Tomczak, and K. Held, Physical Review B 95, 115107 (2017)

O 94.6 Thu 11:45 HL 001

Non-local correlations in effectively reduced spatial dimensions — •Jan M. Tomczak[1], Matthias Pickem[1], Benjamin Klebel[1], Anna Galler[2], Josef Kaufmann[1], Patrik Gunacker[1], Patrik Thunström[3], Thomas Schäfer[2], Alessandro Toschi[1], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, Austria — [2]Centre de Physique Théorique, Ecole Polytechnique, Palaiseau, France — [3]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Using the dynamical vertex approximation and its recent extension for electronic structure calculations, AbinitioDΓA[1], we explore the impact of spatial dimensions onto non-local correlations: (a) we compare magnitude and manifestations of non-local self-energies in ultra-thin films of transition-metal oxides to those in the bulk material. (b) we track the evolution of non-local correlations in the doped Hubbard model when continuously going from 3D to 2D. In particular we probe the limits of the “space-time separation” of electronic correlations evidenced in 3D[2]. Support by the ERC project AbinitioDGA (306447) and the Austrian Science Fund (FWF) projects I 2794-N35 and P 30213-N36 is acknowledged.

References: [1] A. Galler, P. Thunström, P. Gunacker, JMT, K. Held, PRB 95, 115107 (2017), [2] T. Schäfer, A. Toschi, JMT, PRB 91, 121107R (2015)

O 94.7 Thu 12:00 HL 001

Does the optical signature of oxidized polyethylene stem from saturated or unsaturated carbonyl defects? — •Guido Roma[1], Fabien Bruneval[1], and Layla Martin-Samos[2] — [1]DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif sur Yvette, France — [2]CNR-Demokritos, Trieste, Italy

Polyethylene (PE), one of the simplest and most used aliphatic polymers, is generally provided with a number of additives, in particular antioxidants, because of its tendency to get oxidized. Carbonyl defects, a product of the oxidation of PE, are occurring in various forms, in particular saturated ones, known as ketones, where a C=O double bond substitutes a CH_2 group, and various unsaturated ones, i.e., with further missing hydrogens. Many experimental investigations of the optical properties in the visible/UV range mainly attribute the photoluminescence of PE to one specific kind of unsaturated carbonyls, following analogies to the emission spectra of similar small molecules. However, the reason why saturated carbonyls should not be optically detected is not clear. We investigated the optical properties of PE with and without carbonyl defects using perturbative GW and the Bethe-Salpeter equation in order to take into account excitonic effects. We discuss the calculated excitonic states in comparison with experimental absorption/emission energies and the stability of both saturated and unsaturated carbonyl defects. We conclude that the unsaturated defects are indeed the best candidate for the luminescence of oxidized PE, and the reason is mainly due to oscillator strengths.

O 94.8 Thu 12:15 HL 001

Bethe-Salpeter equation beyond the Tamm-Dancoff approximation at finite momentum transfer: Absorption and loss spectra including excitonic effects — •Benjamin Aurich, Caterina Cocchi, and Claudia Draxl — Humboldt-University, Berlin, Germany

The state-of-the-art ab-initio method for computing optical properties of semiconductors is based on the Bethe-Salpeter equation (BSE) which describes the excitations of the system in terms of interacting electron-hole (e-h) pairs. For absorption spectra, typically no momentum transfer from light to the e-h pairs is considered, and the coupling between excitations and de-excitations of e-h pairs is usually neglected by using the Tamm-Dancoff approximation (TDA). This approach yields excellent agreement with experiment for many materials, but may break down for confined systems [1]. The TDA is also known to fail to describe the electron energy loss spectra for materials as simple as silicon [2]. We report on the extensions of the open-source code `exciting` [3] allowing for BSE calculations beyond the TDA and at finite momentum transfer using an exact diagonalization scheme [4]. We demonstrate the differences between TDA and non-TDA spectra at vanishing and finite momentum transfer for periodic molecular systems.

[1] M. Grüning et al., Nano Lett **9**, 2820 (2009)
[2] V. Olevano and L. Reining, Phys. Rev. Lett. **86**, 5962 (2001)
[3] A. Gulans et al., J. Phys. Condens. Matter **26**, 363202 (2014)
[4] T. Sander et al., Phys. Rev. B **92**, 045209 (2015)

O 94.9 Thu 12:30 HL 001

Calculations of charge and spin susceptibilities and quasiparticle energy shifts within the CASTEP plane-wave DFT code — •Vincent Sacksteder[1], Evgeny Plekhanov[2], Phil Hasnip[3], Matt Probert[3], Stewart Clark[4], Keith Refson[1], and Cedric Weber[2] — [1]Royal Holloway University of London, UK — [2]Kings College London, UK — [3]University of York, UK — [4]University of Durham, UK

CASTEP is a pseudopotential based plane wave code which scales to the largest supercomputers and offers a wide feature set. Within CASTEP we have implemented calculation of the charge and spin susceptibility tensor, which describes the response to a perturbing charge or spin. We present corrections to the Kohn-Sham energies obtained by using the susceptibility tensor to screen Hartree-Fock exchange. In the static limit this is the SEX part of the COHSEX approximation, and if instead the dynamic susceptibility is used one obtains the GW approximation.

Our memory and CPU consumption scales linearly with the plane wave basis size, allowing thorough exploration of convergence with basis size, not only of the susceptibility itself, but of the SEX and GW quasiparticle shifts. We emphasize that our calculations are heavily parallelized, in exactly the same way as a standard DFT ground state calculation.

This work will allow first principles calculations of magnon spectra, exchange couplings, ionization potentials, and KKR and DMI coefficients.

O 95: Other And Miscellaneous

Time: Thursday 12:00–13:00 Location: MA 144

O 95.1 Thu 12:00 MA 144

Sub-Pulse Formation and Limit-Cycle Oscillations in an Infrared FEL Oscillator — •Riko Kiessling[1], Sandy Gewinner[1], Wieland Schöllkopf[1], William Bill Colson[2], Martin Wolf[1], and Alexander Paarmann[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Naval Postgraduate School, Monterey, California, USA

Due to their high brightness, ultrashort pulse generation and widely tunable spectral range - from THz photons up to hard X-ray radiation - free-electron laser (FEL) light sources provide unique possibilities for scientific research. Besides that, the FEL itself posseses interesting nonlinear dynamics in the relativistic regime governed by short optical pulses and electron bunches.

Here, we present experimental and theoretical investigations on the sub-pulse formation and limit-cycle oscillations in an infrared FEL oscillator. Cavity shortening is found to be critical for the optical pulse creation. Utilizing a cross-correlation technique with a low-jitter synchronized table-top laser, we observe the build-up and evolution of multiple-peaked FEL pulses, composed of ps-short sub-pulses. The resulting oscillations of the emitted FEL power on a micro-second timescale represent a stable limit-cycle mode of the nonlinear FEL electron-photon system. Our observations are in agreement with predictions based on Maxwell-Lorentz theory [1] and might be of relevance also for recently proposed X-ray FEL oscillators [2].

[1] W. B. Colson, Phys. Quantum Electron. 8, 457 (1982)
[2] K.-J. Kim et al., Phys. Rev. Lett. 100, 244802 (2008)

O 95.2 Thu 12:15 MA 144

Conductance of a Freestanding Conjungated Wire — •Torben Jasper-Tönnies[1], Aran Garcia-Lekue[2,3], Thomas Frederiksen[2,3], Sandra Ulrich[4], Rainer Herges[4], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, 24098 Kiel, Germany — [2]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, Donostia-San Sebastián, Spain — [3]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [4]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität, 24098 Kiel, Germany

A free-standing molecular wire is placed vertically on Au(111) using a platform molecule and contacted by a scanning tunneling microscope. Despite the simplicity of the single-molecule junction its conductance G reproducibly varies in a complex manner with the electrode separation. Transport calculations show that G is controlled by a deformation of the molecule, a symmetry mismatch between the tip and molecule orbitals, and the breaking of a C≡C triple in favor of a Au–C bond. This tip-controlled reversible bond formation and rupture alters the electronic spectrum of the junction and the states accessible for transport, resulting in an order of magnitude variation of the conductance. Financial support by the Deutsche Forschungsgemeinschaft (SFB 677) and the Basque Department of Education (PI-2016-1-0027) is gratefully acknowledged.

O 95.3 Thu 12:30 MA 144

Surface characterisation of bacteria and biofilms with near-ambient pressure X-ray photoelectron spectroscopy — •Marit Kjaervik[1], Paul Dietrich[2], Andreas Thissen[2], Karin Schwibbert[1], and Wolfgang Unger[1] — [1]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany

The XPS information depth of approximately 10 nm is in the same size range as the outer membrane of the gram-negative bacteria, which makes XPS a suitable tool for determining the elemental composition of the bacterial surface and monitor changes caused by outer stress like dehydration or exposure to antimicrobials. However, bacteria are inherently in a hydrated state, and therefore only compatible to ultra-high vacuum after extensive sample preparation, which may degrade the sample constituents. This issue is addressed by the development of near-ambient pressure (NAP)-XPS, which enables bacteria and biofilms to be characterised in their native wet state. Artificial biofilms, bacteria and biofilms of Escherichia coli have been characterised with the laboratory NAP-XPS instrument EnviroESCA from SPECS GmbH, at pressures ranging from high vacuum to 12 mbar, and in both humid and dry environment. By studying biological samples in their native wet state, new insight about composition and transport of drugs through cell membranes and the extracellular polymeric substance (EPS) of biofilms can be obtained. In this contribution, the latest progress on biofilm characterisation by NAP-XPS will be presented, and measurement capabilities and limitations will be discussed.

O 95.4 Thu 12:45 MA 144

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

The arrangement of surface atoms is an important input parameter for density functional theory (DFT) calculations of the electronic structure at the surface. It has been shown that Total Reflection High-Energy Positron Diffraction (TRHEPD) is an ideal technique to determine the structure of the topmost and the immediate subsurface atomic layer of crystal surfaces. In contrast to electrons that are used in Reflection High-Energy Electron Diffraction (RHEED), positrons exhibit the phenomenon of total reflection for glancing angles smaller than the critical angle θc leading to the outstanding surface sensitivity of TRHEPD. Additional information about near-surface layers can be obtained by

increasing the glancing angle above the critical angle.
Currently, we develop a new TRHEPD setup that will be coupled to the high-intensity positron source NEPOMUC in 2018. The TRHEPD setup features UHV down to 10^{-10}mbar, sample temperatures up to 1000°C and a RHEED system for complementary measurements. In combination with the existing Surface Spectrometer (SuSpect), NEPOMUC will provide a unique ensemble to characterize surfaces using positrons. This project is supported by the BMBF (funding number 05K16WO7).

O 96: Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures VI

Organizers: Sabine Maier, FAU Erlangen-Nürnberg; Meike Stöhr, University of Groningen
(Synopsis provided with part I of this session)

Time: Thursday 15:00–18:15 Location: MA 004

O 96.1 Thu 15:00 MA 004

On-Surface Synthesis and Characterization of an Iron Corrole — •Martin Schmid[1], Malte Zugermeier[1], Jan Herritsch[1], Benedikt Klein[1], Claudio Krug[1], Lukas Ruppenthal[1], Philipp Müller[1], Martin Bröring[2], and J. Michael Gottfried[1] — [1]Philipps-Universität Marburg, Fachbereich Chemie, Marburg, Germany — [2]Technische Universität Braunschweig, Institut für Anorganische und Analytische Chemie, Braunschweig, Germany

Tetrapyrrole layers (e.g. porphyrins or phthalocyanines) can be metalated with an on-surface reaction scheme under UHV conditions to obtain the corresponding metallo-tetrapyrroles, in which the metal atoms usually have a +II oxidation state. In order to obtain different oxidation states in the tetrapyrrole films, we examined an alternative class of molecules: corroles. Corroles differ from porphyrins by the absence of one bridging CH unit between two pyrrole units and the presence of a further hydrogen atom in the central pocket of the molecule. Thus, one could expect to find metal atoms in a +III oxidation state. We prepared multilayers and monolayers of 3H-hexaethyl-dimethyl-corrole (3H-HEDMC) on Ag(111) and performed a series of in-situ metalation experiments wit Fe. We analyzed the systems with XPS, UPS, NEXAFS and STM. We find that the corrole ligands can be in-situ metalated and that the iron metal centers are in a +III oxidation state in the multilayer. Additional comparative measurements with Fe(II)-octaethylporphyrin monolayers elucidate differences in the valence electronic structure between Fe(II) and Fe(III) tetrapyrroles on Ag(111).

O 96.2 Thu 15:15 MA 004

On-surface Metalation of the Salophene Ligand and Investigations of local Electronic Properties — •Micha Elsebach[1], Julia Goedecke[1], Emil Sierda[1,2], Marta Przychodnia[2], Maciej Bazarnik[1,2], and Roland Wiesendanger[1] — [1]Dept. of Physics, University of Hamburg, D-20355 Hamburg, Germany — [2]Institute of Physics, Poznan University of Technology, Piotrowo 3, 60-965 Poznan, Poland

Due to their electronic and magnetic properties in combination with their versatility, molecular systems promise high potential for future application in spintronic devices. Previously we showed that Co-salophenes can be used for the fabrication of an all-spin-based logic gate on Au(111) [1]. However, the Co-atoms within the salophene ligand are in the second oxidation state and therefore carry only spin $\frac{1}{2}$. Other metal centers will have a different spin state and therefore might present stronger magnetic coupling within a chain of molecules created by the Ullmann coupling.

The chemical synthesis of complexes based on the salophene ligand in solution is a difficult task that bears the problem of getting a clean sample of the desired complex. Therefore, we performed on-surface metalation of an empty salophene ligand terminated with two H-atoms. During this procedure the creation of counter ions and other secondary products is highly improbable. Here, we present STM and STS studies on the on-surface metalated molecules, and their *ex situ* synthesized counterparts.

[1] M. Bazarnik et al., Nano Lett. 16, 577 (2016).

O 96.3 Thu 15:30 MA 004

On-surface synthesis of Si-porphyrins — •Aleksandr Baklanov, Manuela Garnica, Knud Seufert, and Willi Auwärter — Physik Department E20, Technische Universität München, James Franck Str. 1, 85748 Garching, Germany

On-surface synthesis of non-metal porphyrins is insufficiently explored, although it could open up a possibility to investigate new complexes. Specifically, silicon porphyrins have attracted attention due to their interesting structure and properties [1]. Here we report silicon functionalized tetraphenylporphyrin (Si-TPP) molecules synthesized on a Ag(100) single crystal surface at room temperature in UHV conditions. Self-assembly and electronic properties of Si-TPP were probed by scanning tunneling microscopy/spectroscopy (STM/STS) and X-ray photoelectron (XP) spectroscopy. The N1s XP spectrum of 2H-TPP contains two peaks corresponding to imminic and pyrrolic nitrogen species, whereas in the Si-TPP case only one peak is observed, indicating that all four nitrogen atoms in the macrocycle are chemically identical. A similar behavior is typical for metalloporphyrins [2]. The C1s signal is not affected by the incorporation of Si in the macrocycle. In STM, Si-TPP can be clearly distinguished from 2H-TPP species by additional protrusions at negative sample bias voltages. Furthermore, STS indicates a change of the 2H-TPP LUMO with the Si-complexation.

[1] J. A. Cissell et al., J. Am. Chem. Soc. **127**, 12212 (2005).
[2] A. C. Papageorgiou et al., J. Phys. Chem. C **120**, 8751 (2016).

O 96.4 Thu 15:45 MA 004

On the Adsorption Behavior of Cyano-Functionalized Porphyrins on Cu(111) and Ag(111): from Dimers over Molecular Wires to Ordered Supramolecular Two-Dimensional Aggregates — Michael Lepper[1], Gretel Siglreithmaier[1], Martin Gurrath[2], Bernd Meyer[2], Hans-Peter Steinrück[1], and •Hubertus Marbach[1] — [1]Lehrstuhl für Physikalische Chemie II — [2]Computer-Chemistry-Center; both Universität Erlangen-Nürnberg

We investigate the impact of peripheral cyano functionalization of the well-studied 2H-tetraphenylporphyrin (2HTPP) by scanning tunneling microscopy (STM) and density functional theory (DFT). Interestingly, depending on the number and the geometry of cyano-functionalized phenyl rings, the free-base porphyrins form dimers or 1D-cains after mild annealing on Cu(111). The linking within the dimers and chains is realized by Cu adatoms as evidenced by comparison of STM and DFT [1]. In contrast, the corresponding Cu-porphyrin analogues form peculiar porous highly ordered 2D-islands on Cu(111). On Ag(111), the cyano-functionalized free-base porphyrin molecules assemble into a long-range 2D square order similar to their analogues without cyano functionalization [1]. We will discuss the presented results in regard of the specific roles of molecule-molecule and molecule-substrate interactions, with a particular emphasis on the specific intramolecular conformations [2] and the potential to tailor-make functional molecular architectures. [1] M. Lepper et al., J. Phys. Chem. C, (2017) DOI: 10.1039/C7CC04182A [2] F. Albrecht et al., NanoLett. 16 (2016) 7703; M. Lepper et al., Chemical Communications, 53 (2017) 8207

O 96.5 Thu 16:00 MA 004

Site-Dependent Conformation of Fe-phthalocyanine on Fe/W(001) — •Alexander Schwarz, Josef Grenz, and Roland Wiesendanger — INF, University of Hamburg, Jungiusstr. 11, 20355 Hamburg

Molecules possess many degrees of freedom and are thus able to adsorb on the same surface on different sites, in different orientation and conformations. Here, we present submolecular resolution results obtained with atomic force microscopy in the non-contact mode of operation at low temperatures on well separated Fe-phtalocyanine molecules deposited onto the Fe monolayer on W(001).

The molecules adsorbs with its central Fe atom on hollow-, bridge- and top-sites in different orientations relative to the substrate. Only on hollow sites the molecule appears planar with a fourfold C_4 symmetry and a central protrusion. On the other two adsorptions sites the central region always exhibits a depression and the outer isoindole ligands appear distorted, which results in a reduced symmetry. We will discuss the origin of the distortion and the role of the bonding between the substrate and the central Fe atom of the molecule as well as the importance of the interaction between the nitrogen atoms in the macrocycle and the substrate.

O 96.6 Thu 16:15 MA 004

Digging for silver – surface chemistry of tin(IV)-phthalocyanine-dichloride on Ag(111) — •C. Zwick[1], E. Wruss[2], G. van Straaten[3], M. Gruenewald[1], T. Ueba[4], R. Forker[1], C. Kumpf[3], S. Kera[4,5], E. Zojer[2], and T. Fritz[1] — [1]FSU Jena, Germany — [2]TU Graz, Austria — [3]Forschungszentrum Jülich, Germany — [4]IMS Okazaki, Japan — [5]Chiba University, Japan

The peculiarities of the dye molecule tin(IV)-phthalocyanine-dichloride ($SnCl_2Pc$) originate from its functionalization with Cl atoms above and below the central tin atom. These are expected to crucially impact on interface formation due to the altered chemical reactivity compared to Cl-free phthalocyanines. We report on the monolayer growth of $SnCl_2Pc$ on Ag(111), focusing on the role played by the Cl atoms in terms of structure formation and surface chemistry. By combining state-of-the-art low-temperature scanning probe microscopy (SPM), distortion-corrected low-energy electron diffraction (LEED) and X-ray standing waves (XSW) measurements, an extensive structural characterization could be realized. This includes the lateral and vertical adsorption geometry of the molecules within the adlayer as well as its epitaxial relation to the substrate. Evidence of chemically altered molecules due to a surface reaction was found by means of SPM and photoelectron emission spectroscopy (PES). Simulations based on density functional theory (DFT) support this conclusion. In this regard, one of the most crucial aspects is the partial dechlorination of $SnCl_2Pc$ to SnClPc. Surprisingly, the single remaining Cl atom is penetrating the silver surface, substituting Ag atoms.

15 min. break

O 96.7 Thu 16:45 MA 004

Structural transformation of surface-confined porphyrin networks via addition of Co atoms — •Brian Baker[1], Florian Studener[1], Kathrin Müller[1], Mihaela Enache[1], Nicolas Marets[2], Veronique Bulach[2], Mir Wais Hosseini[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen — [2]Laboratoire de Tectonique Moleculaire, UMR UDS-CNRS 7140, Universite de Strasbourg

The self-assembly process of a nickel-porphyrin (Ni-DPPyP) derivative containing two pyridyl coordinating sites and two pentyl chains at trans meso positions under ultrahigh vacuum on Au(111) was studied with scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED). Deposition of Ni-DPPyP onto Au(111) gave rise to the formation of a close-packed network with a square unit cell as revealed by STM and LEED. The molecular arrangement of this two-dimensional network is stabilized via hydrogen bonds formed between the pyridyl's nitrogen and hydrogen atoms from the pyrrole groups of neighboring molecules. Subsequent deposition of cobalt atoms onto the close-packed network and annealing at 150 degrees celsius lead to the formation of a Co-coordinated hexagonal porous network with a rhombic unit cell. The Co-coordinated network is stabilized by metal-ligand bonds between one cobalt atom and three pyridyl ligands, each pyridyl ligand coming from a different Ni-DPPyP molecule.

O 96.8 Thu 17:00 MA 004

Molecular adsorption of 5, 15-diphenylporphyrin on CoO (111) films — •Feifei Xiang and M. Alexander Schneider — Solid State Physics, Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Erlangen, Germany

The adsorption geometry of 5, 15-diphenylporphyrin (2H-DPP) on a ~2.7 nm thick CoO (111) film is studied by low temperature scanning tunneling microscopy. Although CoO is a semiconductor, the oxygen terminated CoO (111) film shows metallic properties according to scanning tunneling spectroscopy data.[1] When deposited at 170 K, 2H-DPP adsorbs as single, flat-lying molecules on the surface due to the hydrogen bonding between the molecule and the surface.[2] With annealing of the molecular adsorbate system, 2H-DPP starts to have reactions with the oxide surface, causing the characteristic changes of its configuration from the original oval shape to a bean shape and eventually to a symmetric feature with reduced apparent molecular width at 470K. From comparison with Co-DPP deposited on CoO (111), we conclude that 2H-DPP gets metalated at around room temperature.

[1] Meyer, W., et al. Phys. Rev. Lett., 2008, 101, 016103.
[2] Wang, C., Chem. Commun., 2014, 50, 8291-8294.

O 96.9 Thu 17:15 MA 004

Porphyrins at surfaces: effect of film formation on the electronic levels — Osman Baris Malcioglu and •Michel Bockstedte — Chemistry and Physics of Materials, University of Salzburg, Salzburg, Austria

Porphyrins on surfaces are used successfully in various applications such as surface catalysis, lighting and energy harvesting. In order to unravel electronic and photophysical properties of such porphyrin films on surfaces, one first has to identify the contribution of the film's supramolecular network. Here, we investigate quasiparticle spectrum of amorphous and crystalline porphyrin structure as a model for supramolecular films of H2TPP and MgTPP. We use VdW-DFT and sc-GW approaches (calibrated against NIST data). We show that the crystalline model agrees with the UPS/2PPE spectra [1] better than individual molecules or other porphyrin structures regarding the position of the HOMO and LUMO state. The interaction of the phenyl rings has strong influence one the position and dispersion of quasiparticle levels of the prophyrin film. Our findings confirm that the systematic control of the film crystallisation or the substitution of residues enables an improvement or tuning of the electronic states and thus leads to better performance of devices [3].

[1] A. Classen, et al., Phys. Rev. B **95**, 115414 (2017).
[2] M. Gamboa, M. Campos, and L.A. Torres, J. Chem. Thermodynamics **42**, 666 (2010)
[3] A. Charisiadis *et al.*, ChemPlusChem, **82**, (2017).

O 96.10 Thu 17:30 MA 004

Charge state control of F_{16}CoPc on *h*-BN/Cu(111) — •Mathias Pörtner[1], Yinying Wei[2], Alexander Riss[1], Knud Seufert[1], Manuela Garcia[1], Johannes V. Barth[1], Lars Diekhöner[2], and Willi Auwärter[1] — [1]Physik-Department E20, Technische Universität München, James-Franck-Str. 1, D-85748 Garching, Germany — [2]Department of Physics and Nanotechnology, Fredrik Bajers Vej 5, DK-9100 Aalborg, Denmark

Molecules on metal supported hexagonal boron nitride (*h*-BN) are of great interest as far as their electronic properties and self-assemblies are accessible by scanning probe methods [1]. Here, we report on the control of the charge state of F_{16}CoPc on atomically thin *h*-BN on Cu(111) studied by low temperature scanning tunneling microscopy and spectroscopy. In the submonolayer regime, molecules adsorb on pore areas of the work-function template *h*-BN/Cu(111) [2]. Tunneling spectroscopy shows that the charge state of F_{16}CoPc can be controlled by three parameters: (i) template-induced gating by the work-function variation of *h*-BN/Cu(111) [2], (ii) field-induced gating by the STM tip [3] and (iii) screening, which depends on the neighboring molecules [4]. These parameters influence the properties of the molecular layer and thus its (templating) functionality. For example the preferred adsorption positions of second layer molecules differ from the first layer.

[1] Kumar, et al., Nanotechnology **28**, 082001 (2017).
[2] Joshi, et al., ACS Nano **8**, 430 (2014).
[3] Liu, et al., ASC Nano **9**, 10125 (2015).
[4] Cochrane, et al., Nat. Commun. **6**, 8312 (2015).

O 96.11 Thu 17:45 MA 004

Apparent reversal of molecular orbitals reveals entanglement — Ping Yu[1,2], Nemania Kocic[1], Benjamin Siegert[3], Jascha Repp[1], and •Andrea Donarini[3] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]School of Physical Science and Technology, ShanghaiTech University, 201210 Shanghai, China — [3]Institute of Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany

The frontier orbital sequence of individual dicyanovinyl-substituted oligothiophene molecules is studied by means of scanning tunneling microscopy. On NaCl/Cu(111) the molecules are neutral, and the two lowest unoccupied molecular states are observed in the expected order of increasing energy. On NaCl/Cu(311), where the molecules are negatively charged, the sequence of two observed molecular orbitals is reversed, such that the one with one more nodal plane appears lower in energy. These experimental results, in open contradiction with a single-particle interpretation, are explained by a many-body theory predicting a strongly entangled doubly charged ground state.

O 96.12 Thu 18:00 MA 004

Magnetism of Salophene based molecules — •Emil Sierda[1,2], Micha Elsebach[1], Maciej Bazarnik[1,2], and Roland Wiesendanger[1] — [1]Department of Physics, University of Hamburg, Jungiusstrasse 11, D-20355, Hamburg, Germany — [2]Institute of Physics, Poznan University of Technology, Piotrowo 3, 60-965, Poznan, Poland

Advances in molecular spintronics rely on the in-depth characterization of the molecular building blocks in terms of their electronic and magnetic properties. For this purpose inert substrates are required that will interact only weakly with adsorbed molecules in order to preserve their electronic states. Magnetic substrates, on the other hand, are useful for stabilizing the magnetic moment of a molecule, thereby making it accessible for investigations by spin-polarized scanning tunneling microscopy (SP-STM) [1].

Here, we present a SP-STM study of Salophene-based molecules with different transition metal centers adsorbed on Co-intercalated graphene on Ir(111) [2]. This substrate is an ideal choice for a thorough characterization of the molecules* electronic and magnetic states. In particular, such studies reveal the differences in magnetic structure between molecules with different transition metal centers. Based on these insights the most promising molecules in view of future molecular spintronic devices can be identified.

[1] Schwöbel, J. et al. Nat. Comm. 3, 953 (2012). [2] Decker R. et al. Phys. Rev. B 87, 041403 (2013).

O 97: Scanning probe techniques: Method development II

Time: Thursday 15:00–18:30 Location: MA 005

O 97.1 Thu 15:00 MA 005

Nanosecond time resolution in Electrostatic Force Microscopy — •Riccardo Borgani, Daniel Forchheimer, Per-Anders Thorén, and David B. Haviland — Nanostructure Physics, KTH Royal Institute of Technology, Stockholm, Sweden

We introduce a scanning probe microscopy technique based on nonlinear electrostatic interaction to map the fast response of a surface to an electric or luminous stimulus. The technique allows for investigation of the fast generation and recombination of charge, e.g. in photo-voltaic materials.

We excite the probe at its resonance frequency, and the material under study with a periodic train of sharp pulses. We drive the cantilever and monitor its deflection near its mechanical resonance frequency, where a high SNR measurement of intermodulation between the drive and the material response to the pulses is possible. The proposed technique is able to reconstruct the rise and fall time of the material response from hundreds of milliseconds to the nanosecond regime.

We show experimental data demonstrating this time resolution, and we discuss the theory and simulations that suggest a even faster time resolution is achievable at the expense of the measurement time. Our work demonstrates how the intermodulation spectral technique, where phase-coherent down-conversion is measured at many frequencies, is an attractive alternative to pump-probe measurements for probing fast dynamics.

O 97.2 Thu 15:15 MA 005

Two-degree-of-freedom control combining machine learning and extremum seeking for fast scanning quantum dot microscopy — •Michael Maiworm[1], Christian Wagner[2,3], Ruslan Temirov[2,3], F. Stefan Tautz[2,3], and Rolf Findeisen[1] — [1]Institute for Automation Engineering (IFAT), Otto-von-Guericke Universität Magdeburg, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [3]JARA-Fundamentals of Future Information Technology, Jülich, Germany

Scanning Quantum Dot Microscopy (SQDM) is a novel technique for the quantitative imaging of surface potential distributions with nanometer resolution[1,2]. The SQDM sensor is a molecular quantum dot (QD) attached to the tip of a non-contact AFM by molecular manipulation. Surface potential variations can change the QD charge state via gating which causes sharp dips in NC-AFM $\Delta f(V_{bias})$ spectra. Mapping of the surface potential is thus possible via mapping of the V_{bias} values at which the respective dips appear. For this purpose we present a two-degree-of-freedom control approach, consisting of an extremum seeking controller and a feedforward control. The feedforward signal is based on a machine learning approach where a Gaussian process is used to capture the already scanned part of the image and compute a prediction for the next scan lines. The proposed control approach speeds up the scanning process by one order of magnitude and enables to scan large areas and strong potential variations. [1] C. Wagner et al. Phys. Rev. Lett. 115, 026101 (2015) [2] M. Green et al. Japan. J. Appl. Phys. 55, 08NA04-7 (2016)

O 97.3 Thu 15:30 MA 005

Mapping Light-Induced Cantilever dynamics by Scanned Laser Radiation — •Sven Kraft, Dieter Schick, Semjon Köhnke, Boris Hage, Ingo Barke, and Sylvia Speller — University of Rostock, Institute of Physics, 18051 Rostock, Germany

Direct actuation of Atomic Force Microscopy (AFM) cantilevers by a laser beam is an alternative method to the widely used dither piezo actuator. In particular in the case of liquid environments laser actuation is beneficial because spurious oscillation modes, visible as the so called "Forest of peaks" [1], are avoided. Our aim is to better understand the mechanisms leading to the laser-induced oscillation, by revealing the dependence of the location of the laser spot on the cantilever. Analysis of spatially and frequency resolved data of different cantilevers indicate that a combination of mechanisms contributes to the total motion. Among them are thermal effects [2,3] and instantaneous forces from radiation pressure [4]. Besides these two we observe quasi-instantaneous thermal actuation forces for coated as well as uncoated cantilevers. The results may allow improved actuation schemes, reducing undesired effects such as cantilever heating.

[1] T. E. Schäffer, J. P. Cleveland, F. Ohnesorge, D. A. Walters, and P. K. Hansma, J Appl Phys 80, 3622 (1996)

[2] D. Ramos, J. Tamayo, J. Mertens, and M. Calleja, J Appl Phys 99, 124904 (2006)

[3] D. Kiracofe, K. Kabayashi, A. Labuda, A. Raman, H. Yamada, Review of Scientific Instruments 82, 013702 (2011)

[4] D. Kleckner, D.Bouwmeester, Nature 444(7115) (2006)

O 97.4 Thu 15:45 MA 005

Molecular model of a quantum dot junction beyond the constant interaction approximation — •Ruslan Temirov[1,2], Niklas Friedrich[1,2], Taner Esat[1,2], Philipp Leinen[1,2], Matthew F. B. Green[1,2], Christian Wagner[1,2], Pawel Chmielniak[3,4,2], Jeffrey Rawson[3,4,2], Paul Kögerler[3,4,2], Michael Rohlfing[5], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA)–Fundamentals of Future Information Technology, Jülich, Germany — [3]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Germany — [4]Institute of Inorganic Chemistry, RWTH Aachen, Germany — [5]Institute for Solid-state Theory, University of Münster, Germany

We present a physically intuitive model of molecular quantum dots beyond the constant interaction approximation. It accurately describes their charging behaviour and allows the extraction of important molecular properties that are otherwise experimentally inaccessible. The model is applied to data recorded with a non-contact atomic force microscope (AFM) on three different molecules that act as a quantum dot when attached to the microscope tip [1-2]. Results are in excellent agreement with first principle simulations.

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

O 97.5 Thu 16:00 MA 005

Intermodulation gain and noise squeezing in dynamic AFM — •David Haviland, Alexander Revera-Ahlin, Daniel Forchheimer, Riccardo Borgani, Thomas Weissl, and Shan Jolin — Nanostructure Physics, KTH, Stockholm, Sweden

When driven by a strong pump, a nonlinear oscillator will create correlations in the frequency domain between signal and idler pairs symmetrically placed about the pump frequency. These correlations result in two-mode squeezing, giving power gain to a weak signal by amplifying one quadrature while the other quadrature is de-amplified. Not only signals but also noise can be squeezed, resulting in measurement sensitivity below the standard limits imposed by thermal or quantum fluctuations. There is currently numerous experiments demonstrating these effects at the quantum limit, but much less attention has been paid to the squeezing of thermal noise where there is in fact great potential for practical applications. We demonstrate parametric gain and thermal noise squeezing in a room-temperature dynamic Atomic Force Microscopy, where the limiting noise is thermal Brownian motion of the cantilever. Unlike previous work on the mechanical amplification of force, we do not use an 'external' nonlinearity to realize gain, but rather the sample itself is used as the 'gain medium'. We show how parametric gain results in a widening of the measurement bandwidth over which dynamic AFM is limited by thermal noise.

O 97.6 Thu 16:15 MA 005

Application of machine learning techniques to multifrequency AFM — •Daniel Forchheimer[1,2], Per-Anders Thoren[1], Riccardo Borgani[1], and David Haviland[1,2] — [1]The Royal Institute of Technology (KTH), Stockholm Sweden — [2]Intermodulation Products AB, Segersta, Sweden

Thanks to the development of multifrequency AFM techniques datasets obtain with scanning probe microscopy are becoming increasingly high-dimensional. With Intermodulation AFM for example, one is able to measure at over 40 frequencies simultaneously, to obtain over 80 "observables" for each image pixel. We have developed extensive analysis methods based on careful modeling and calibration of the AFM system, to convert these raw observables to interpretable physical properties.

However, this analysis can be quite computationally intense, and in some situations not even possible, as for example the case of broad band interaction where multiple eigenmodes are excited where calibration is lacking. Therefore it is also of interest to apply tools from "big data analysis", i.e. machine learning tools such as clustering and dimensionality reduction where analysis is performed on the raw observables, agnostic to the physical system. We have applied some machine learning algorithms to multifrequency AFM to investigate its utility and to compare with an the results of physical modeling.

15 min. break

O 97.7 Thu 16:45 MA 005

Low temperature scanning tunneling microscope with optical access — •Lars Wilmes[2], Kevin Edelmann[1,2], Moritz Winkler[2], Lukas Gerhard[2], and Wulf Wulfhekel[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruher Institut für Technologie, 76344 Eggenstein-Leopoldshafen, Germany

Exploring the conversion of electric power to light and the relevant processes at a molecular level is key for the further development and miniaturization of high efficient light emitting devices. Systematic investigations with a reduced number of degrees of freedom can be achieved in single molecule junctions in a scanning tunneling microscope (STM). A new ultra high vacuum low temperature (1.5 K) STM featuring an optical access with high collection efficiency gives experimental access to plasmons within the tunnel junction and electroluminescence from single molecules. A silver coated tip within a microscopic parabolic mirror is used to focus light directly into an optical fiber. With a single fiber to guide the collected light into a spectrometer the STM provides a combination of optical and electrical spectroscopy. Preliminary results show promising photon yield with atomic-scale spatial resolution.

O 97.8 Thu 17:00 MA 005

Evaluating the potential energy above a single molecule at room temperature with lateral force microscopy — •Alfred J. Weymouth, Elisabeth Riegel, Sonia Matencio, and Franz J. Giessibl — Universität Regensburg, Regensburg, Germany

One of the challenges of AFM, in contrast to STM, is that the measured signal includes both long-range and short-range components. The most accurate method for removing long-range components is to measure both on and off an adsorbate and to subtract the difference. [1] This on-off method, however, is challenging at room temperature due to thermal drift. By moving to a non-contact scheme in which the lateral component of the force interaction is probed, the measurement is dominated by short-range interactions. [2] We use non-contact lateral force microscopy (LFM) in the frequency-modulation mode and measure the local interaction above a PTCDA island grown on Ag/Si(111)-($\sqrt{3} \times \sqrt{3}$). Each molecule appears as a single feature. By fitting this feature to a model potential, we can extract the depth and width of the potential. As we move closer to the sample, we reach the range in which Pauli repulsion plays a role in our tip-sample interaction.

[1] Ternes et al., Phys. Rev. Lett. 106, 016802 (2011)
[2] Weymouth, J. Phys. Condens. Matter. 29, 323001 (2017)

O 97.9 Thu 17:15 MA 005

Unexpected lateral contrast in Topografiner imaging on sub-Angström corrugations — •Gabriele Bertolini[1], Robin Pröbsting[1], Danilo Andrea Zanin[1], Hugo Cabrera[1], Urs Ramsperger[1], Danilo Pescia[1], and Oguzhan Gürlü[1,2] — [1]Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland — [2]Auguste-Piccard-Hof 1, HPT C5.3 ETH Hoenggerberg

By running the Scanning Tunnelling Microscope (STM) in the Fowler-Nordheim regime, i.e. going back to Topografiner from STM, we were able to attain lateral resolution with several nanometers on structures embedded in W(110) terraces, which have less than 20 pm corrugation. Our results showed that local work function on the surface is modified at the atomic level due to contaminants as expected, and this is reflected in the imaging capability of Topografiner with such unexpected lateral resolution. The secondary electron (SE) images and absorbed current images present complementary information. This in itself showed the extreme sensitivity of this imaging technique to local chemical environment. Furthermore our results showed that SEs dominate the signal reaching to the detector from the tip-sample junction rather than elastically back scattered electrons.

O 97.10 Thu 17:30 MA 005

Coherent single electron field emitter assembled with SPM — •Taner Esat[1,2], Niklas Friedrich[1,2], Ruslan Temirov[1,2], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, Germany

In this work we demonstrate the assembly of a coherent single electron field emitter by controlled manipulation of individual atoms and a molecule with the tip of a combined NC-AFM/STM.

O 97.11 Thu 17:45 MA 005

Investigation of the significance of higher harmonics in non-contact atomic force microscopy — •Daniel Heile, Alexander von Schmidsfeld, and Michael Reichling — Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück

In the non-contact atomic force microscopy the prevalent theoretical approach to force sensor oscillations is the harmonic approximation. Hence, the complex cantilever oscillations are simplified to a harmonic oscillator at its tip position. This is a sufficient approximation for a cantilever in the freely oscillating case. However, for applied loads on the cantilever, for example due to tip-sample interactions, higher harmonic cantilever modes occur. To describe the dynamics of the cantilever we introduce the finite differences method (FDM) on the basis of the Euler-Bernoulli beam theory. This numerical approach allows the detailed description of the cantilever dynamics under applied loads and hence provides information on the modal structure and frequency spectrum. With that approach the deviation of the tip movement from the sinusoidal harmonic oscillation can be investigated in detail.

O 97.12 Thu 18:00 MA 005

Information content comparison of mulitfrequency afm methods — •Daniel Platz[1], Daniel Forchheimer[2], Erik Tholén[3], and David B. Haviland[2] — [1]TU Wien, Gußhausstraße 27-29, A-1040 Vienna, Austria — [2]KTH Royal Institute of Technology, Albanova University Center, SE-106 91 Stockholm, Sweden — [3]Intermodulation Products AB, Landa Landavägen 4193, SE-823 93 Segersta, Sweden

Dynamic atomic force microscopy (AFM) is one of the key tools for imaging and measuring matter at the nanoscale. In conventional dynamic AFM a small tip at the end of a micro-cantilever oscillates at one frequency above a sample surface. In recent years, several multifrequency methods have been developed to increase the information content of AFM measurements. All these multifrequency methods allow for tip motion comprising multiple frequency components but they are based on different principles like the excitation of multiple cantilever eigenmodes, measurement of higher harmonics of the tip motion or creation of spectral mixing products. Although multifrequency methods have been extensively studied experimentally, it is not well understood how different methods compare. We developed a framework for the consistent comparison of multifrequency AFM methods. The framework is based on the numerical kernel estimation method which allows for an easily understandable interpretation of spectral frequency components. Using this approach, we are able to quantify the information content of different multifrequency AFM methods and to study their robustness to noise.

O 97.13 Thu 18:15 MA 005

Characterising NC-AFM cantilevers by opto-mechanical forces — •Alexander von Schmidsfeld and Michael Reichling — Universität Osnabrück

Cantilevers are harmonic oscillators that are designed to have a high sensitivity for the detection of minute external forces typically used in non-contact force microscopy (NC-AFM) to detect forces originating from the tip-sample interaction.

We use opto-mechanical forces acting in the light field of an interferometer for measuring the displacement of an oscillating cantilever for a complete characterization to derive the eigen-frequency (f_0), Quality-factor (Q) oscillation amplitude (A) and cantilever stiffness (k_0) of the cantilever.

As the radiation pressure acting on the cantilever can be determined and the interferometer provides a precise, intrinsically calibrated displacement measurement, these for the interpretation of NC-AFM images crucial properties can be determined with remarkable precision. Due to the sinusoidal intensity modulation of the light intensity an amplitude dependent frequency shift is observed enabling the comparison of the opto-mechanical force to the restoring force. By exactly characterizing the interferometer the light intensity inside the cavity formed by fiber and cantilever and thus the opto-mechanical force can be determined with high precision.

O 98: Electronic structure: Surface magnetism and spin phenomena I

Time: Thursday 15:00–18:30 Location: MA 042

O 98.1 Thu 15:00 MA 042

Long spin relaxation time in a transition metal atom in contact to a metal substrate — Jan Hermenau[1], Markus Ternes[2], •Manuel Steinbrecher[1], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Department of Physics, Hamburg University, 20355 Hamburg, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Long spin-energy relaxation times are a prerequisite for the use of spins in data storage or nanospintronics technologies. An atomic-scale solid-state realization of such a system is the spin of a transition metal atom adsorbed on a suitable substrate. For the case of a metallic substrate, which enables a direct contacting of the spin by conduction electrons, the lifetimes reported to date are extremely short and on the order of only hundreds of femtoseconds [1,2]. Here, we show that the spin states of iron atoms adsorbed directly on a conductive platinum substrate have an astonishingly long spin-energy relaxation time in the nanosecond regime, which is comparable to that of a transition metal atom which is decoupled from the substrate electrons by a thin decoupling layer [4]. The combination of long spin-energy relaxation times and strong coupling to conduction electrons implies the possibility to use flexible coupling schemes in order to process the spin-information.
[1] A. A. Khajetoorians *et al.*, PRL **111**, 157204 (2013)
[2] T. Schuh *et al.*, J. Appl. Phys. **107**, 09E156 (2010)
[4] W. Paul *et al.*, Nat. Phys. **13**, 403 (2017)

O 98.2 Thu 15:15 MA 042

Engineering the couplings in atomically crafted spin chains on elemental superconductors — •Anand Kamlapure, Lasse Cornils, Jens Wiebe, and Roland Wiesendanger — Department of Physics, University of Hamburg, Hamburg, Germany

Spin chains coupled to s-wave superconductors realized by linear arrays of transition metal atoms on the surface of elemental superconductors may lead to topological superconductivity accompanied by the emergence of Majorana zero modes at the chain ends [1-3]. For realizing braiding of Majonara zero modes, which is ultimately needed for their usage in quantum computation, it is a prerequisite to artificially assemble such chains as well as control the exchange coupling between the chain atoms.
Here, we artificially create chains of different numbers of Fe adatoms [4] and interstitial Fe atoms on an oxygen reconstructed Ta(100) substrate using the tip of a scanning tunneling microscope as a tool. We find that the interaction within the chain can be strengthened by linking the Fe adatoms with interstitial Fe atoms, adding an important step towards the controlled design of quantum circuits employing Majorana end states.
[1] S. Nadj-Perge et al., Phys. Rev. B **88**, 020407(R) (2013).
[2] F. Pientka et al., Phys. Rev. B **88**, 155420 (2013).
[3] J. Klinovaja et al., Phys. Rev. Lett. **111**, 1 (2013).
[4] L. Cornils et al., Phys. Rev. Lett. **119**, 197002 (2017).

O 98.3 Thu 15:30 MA 042

Optically and Electrically Controllable Adatom Spin-orbital Dynamics in Transition Metal Dichalcogenides — Bin Shao[1,2], •Malte Schueler[1,2], Gunnar Schönhoff[1,2], Thomas Frauenheim[2], Gerd Czycholl[1], and Tim Wehling[1,2] — [1]Institute for theoretical Physics, University of Bremen, Bremen, Germany. — [2]Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany.

We analyze the interplay of spin-valley coupling, orbital physics, and magnetic anisotropy taking place at single magnetic atoms adsorbed on semiconducting transition metal dichalcogenides, MX_2 (M = Mo, W; X = S, Se). Orbital selection rules turn out to govern the kinetic exchange coupling between the adatom and charge carriers in the MX_2 and lead to highly orbitally dependent spin-flip scattering rates, as we illustrate for the example of transition metal adatoms with d^9 configuration. Our ab initio calculations suggest that d^9 configurations are realizable by single Co, Rh, or Ir adatoms on MoS_2, which additionally exhibit a sizable magnetic anisotropy. We find that the interaction of the adatom with carriers in the MX_2 allows to tune its behavior from a quantum regime with full Kondo screening to a regime of "Ising spintronics" where its spin-orbital moment acts as classical bit, which can be erased and written electronically and optically.

O 98.4 Thu 15:45 MA 042

Probing surface magnetism with a nickelocene tip — •Benjamin Verlhac[1], Nicolas Bachellier[1], Léo Garnier[1], Maider Ormaza[1], Paula Abufager[2], Nicolás Lorente[3], Markus Ternes[4], Marie-Laure Bocquet[5], and Laurent Limot[1] — [1]Université de Strasbourg, CNRS, IPCMS, Strasbourg, France — [2]Instituto de Física de Rosario-CONICET-Universidad Nacional de Rosario,Rosario, Argentina — [3]Donostia International Physics Center (DIPC), San Sebastián, Spain — [4]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [5]ENS-CNRS-UPMC, Paris, France

Inelastic electron tunneling spectroscopy (IETS) within the junction of a scanning tunneling microscope (STM) uses current-driven spin excitations for an all electrical characterization of the spin state of a single object. Here we study the magnetism of a sandwich nickelocene molecule (Nc) adsorbed on Cu(100) by means of X-ray magnetic circular dichroism (XMCD) and density functional theory calculations (DFT), and show with IETS that it exhibits efficient spin excitations. The molecule preserves its magnetic moment and magnetic anisotropy not only on Cu(100), but also in different metallic environments including the tip apex. Taking advantage of this robusteness, we use a functionalized Nc tip to detect the magnetism of a single Fe adatom.

O 98.5 Thu 16:00 MA 042

Controled spin switch in a nickelocene molecular junction — •Benjamin Verlhac[1], Maider Ormaza[1], Nicolas Bachellier[1], Paula Abufager[2], Marie-Laure Bocquet[3], Nicolás Lorente[4], and Laurent Limot[1] — [1]Université de Strasbourg, CNRS, IPCMS, Strasbourg, France — [2]Instituto de Física de Rosario-CONICET-Universidad Nacional de Rosario,Rosario, Argentina — [3]ENS-CNRS-UPMC, Paris, France — [4]Donostia International Physics Center

(DIPC), San Sebastián, Spain

One of the main challenges in molecular spintronics is to achieve an active control of a molecular spin. This is possible through the modification of the molecular structure either by chemical doping or by external stimuli. Here we investigate the effect of varying the electrode-electrode distance in a controled way in a single nickelocene molecular junction using a low-temperature scanning tunneling microscope. The molecule, when attached to the metallic tip of the microscope, exhibits spin excitations in the tunneling regime, while a Kondo ground state emerges upon contact with a Cu(100) surface, causing then an order of magnitude change in the zero-bias conductance. First principle calculations show that nickelocene reversibly switches from a spin 1 to 1/2 between the two transport regimes.

O 98.6 Thu 16:15 MA 042

Spin-resolved electron transmission through self-assembled layers of PNA — •Paul Möllers[1], Daniel Nürenberg[1], Matthias Kettner[1], Francesco Tassinari[2], Tal Markus[2], Selma Ulku[3], Catalina Achim[3], Ron Naaman[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Chemical Physics, Weizmann Institute, Rehovot, Israel — [3]Department of Chemistry, Carnegie Mellon University, Pittsburgh, United States

The yield of electrons transmitted through chiral molecules can depend on the electron's spin; chiral molecules can therefore act a spin filters. This effect is referred to as the chirality-induced spin selectivity (CISS) effect. Previous experiments have e.g. been performed with monolayers of double-stranded DNA [1]. In this contribution, we present results of our spin-resolved photoemission experiments performed at room temperature. The samples consist of self-assembled monolayers of helical molecules – various types of double-stranded peptide nucleic acid (PNA) – on polycrystalline gold surfaces. The samples are irradiated by a laser at $\lambda = 213\,\mathrm{nm}$ to generate photoelectrons from the gold substrate which are then transmitted through the adsorbed monolayer. Subsequently, the electrons are analyzed by a Mott polarimeter. We found longitudinal spin polarizations of $-6\,\%$ for PNA and $+25\,\%$ for γ-PNA. The results indicate that the adsorbed molecules act as a spin filter.

[1] B. Göhler et al., Science 331, 894 (2011)

15 min. break

O 98.7 Thu 16:45 MA 042

Inelastic Spin- and Vibrational Excitations on FeTPyP on Au(111) — •Daniela Rolf[1], Friedrich Maass[2], Christian Lotze[1], Benjamin W. Heinrich[1], Constantin Czekelius[3], Petra Tegeder[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin — [2]Universität Heidelberg — [3]Heinrich-Heine Universität Düsseldorf

Porphyrin molecules constitute a class of well-investigated molecules, because of their versatility in terms of self-assembly and electronic and magnetic properties. Numerous studies have been performed with various central metal atoms on different metal surfaces, showing that by a suitable choice of metal center and surface, the molecular properties can be tailored. Interesting phenomena were observed, including the Kondo effect, vibronic coupling and negative-differential resistance. Here, different arrangements of Fe-tetra-pyridil-porphyrin (Fe-TPyP) molecules were investigated on a Au(111) substrate. Employing a low-temperature STM, we show that depending on the molecular geometry, a different number of steps in the dI/dV signal can be observed symmetrically around the Fermi level, with energies up to 115meV. Comparison to HREELS measurements allows for an unambigous identification of vibrational excitations. The lowest energy steps correspond to spin excitations. We correlate the variations in the spectral features to different magnetic ground states and d-level alignments originating from distinct molecular configurations of the self-assembled structures.

O 98.8 Thu 17:00 MA 042

Yu-Shiba-Rusinov states of magnetic adatoms on the quasi 2D superconductor $2H$-NbSe$_2$ — •Eva Liebhaber[1], Rojhat Baba[1], Lisa Rütten[1], Michael Ruby[1], Sebastian Rohlf[2], Kai Rossnagel[2], Benjamin W. Heinrich[1], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany. — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany.

A magnetic impurity adsorbed on a superconducting substrate yields so-called Yu-Shiba-Rusinov (YSR) states. These are low energy bound states inside the superconducting energy gap locally induced by magnetic exchange scattering. $2H$-NbSe$_2$ belongs to the class of transition metal dichalcogenides and is a layered van der Waals material with strong 2D character. In this material, superconductivity coexists with a charge density wave (CDW) at low temperatures.

Here, we investigate YSR states of single transition metal atoms adsorbed on the surface of $2H$-NbSe$_2$ using low temperature scanning tunneling microscopy and spectroscopy. We observe variations in d state resonances as well as in the YSR excitations. We can link these variations to the adsorption in two distinct atomic sites. Furthermore, the energy of the YSR states and their spatial extend appear to be influenced by the CDW.

O 98.9 Thu 17:15 MA 042

Magnetic Vortex Core Pinning at Atomic Scale Surface Perturbations — •Christian Holl[1], Marvin Knol[1], Marco Pratzer[1], Imara L. Fernandes[2], Jonathan Chico[2], Samir Lounis[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52428 Jülich, Germany

Spin polarized scanning tunneling microscopy is used to observe magnetic pinning centers in sub micrometer sized iron platelets. The magnetic ground state of these platelets is a flux closed magnetic vortex whose core can be moved laterally by in-plane magnetic fields[1]. Despite their small volume compared to the vortex core, we show that the core pins to the individual surface adsorbates, presumably oxygen, if the core is squeezed by a perpendicular magnetic field of 1.5 T. Comparison with micro-magnetic simulations reveal a pinning energy of up to 250 meV induced by a single adsorbate. *Ab initio* based calculations show that oxygen adatoms induce anisotropic exchange interactions in the neighbouring substrate atoms[2], which explains the non-concentric pinning position of the core.

[1] A. Wachowiak et al., Science **298**, 577-580 (2002)
[2] Funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 - DYNASORE).

O 98.10 Thu 17:30 MA 042

Spin-orbit gaps in ferromagnetic thin films — •Lukasz Plucinski[1], Ewa Mlynczak[1], Stephan Borek[2], Jan Minar[2], Jürgen Braun[2], Mathias Gehlmann[1], Irene Aguilera[3], Gustav Bihlmayer[3], Stefan Blügel[3], Hubert Ebert[2], and Claus M. Schneider[1] — [1]PGI-6, FZ Jülich — [2]LMU, Munich — [3]PGI-1, FZ Jülich

Magnetization direction can control topological phases in ferromagnets by influencing the existence of nodal points and spin-orbit gaps, which control intrinsic magnetotransport properties. Using high resolution angle-resolved photoemission we demonstrate openings of spin-orbit gaps, near the Fermi level [PRX 6, 041048 (2016)]. The gaps and thus the Fermi surface could be manipulated by changing the remanent magnetization direction, and we find qualitative agreement to the one-step model photoemission calculations. For thinner films the quantum confinement leads to quantum wells which also exhibit anisotropy. The analysis of spin-polarized photoemission from these quantum wells allows the unambiguous identification of the initial bands, which has been often challenging due to correlation effects in the band structure, which are beyond the description of popular exchange-correlation potentials. Good agreement is found by comparison to the bulk band structure calculated using the GW method under the assumption of perpendicular momentum broadening due to the finite probing depth of photoemission. This study contributes to better understanding of the role of Berry phase physics in anomalous Hall conductivity and related phenomena in 2D ferromagnetic layers.

O 98.11 Thu 17:45 MA 042

Orbital magnetism of $3d$ adatoms deposited on transition metal surfaces — •Sascha Brinker, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich

The classical definition of the orbital magnetic moment using the ground state charge current is well-defined for finite systems, while for periodic systems the modern theory of orbital magnetization applies. In this work we consider the intermediate case: small magnetic nanostructures deposited on surfaces from first-principles. As an application we consider $3d$ transition metal adatoms deposited on different transition metal surfaces, e.g. Ir(111), Pt(111) and Au(111), and their ground state charge current distributions. We find two contributions to the orbital magnetic moment: a local contribution corresponding to the swirling charge currents around each atom and a non-local contribution related to the net currents flowing between atoms. We show that the non-local contribution, which was neglected in previous works, is an important part of the total orbital magnetic moment, and can even exceed the local contribution. Our findings can be relevant for future experiments with nano-diamonds [1] and ESR-STM [2].

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

[1] L. Rondin *et al.*, *Rep. Prog. Phys.* **77**, 056503 (2014)
[2] S. Baumann *et al.*, *Science* **350**, 417-420 (2015)

O 98.12 Thu 18:00 MA 042

Fe/Rh(111): a magnetic ground state driven by higher-order spin interactions — Markus Hoffmann, •Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Although for $S > \frac{1}{2}$ systems higher order spin interactions can be expected to get important, the magnetism of transition metals is often studied in the (classical) Heisenberg model. Surprisingly, the two-spin interactions from this model describe many systems rather well, only in some cases biquadratic or cyclic four-spin terms have to be added. Here, we present the system of one monolayer Fe on Rh(111) where an even more exotic term, a 3-site 4-spin interaction, is necessary to explain the ground state that was predicted by density functional theory [1] and recently confirmed experimentally [2]. The Fe layer shows a double–row-wise antiferromagnetic structure, that can be described as double-$\mathbf{Q}$ state. Another double-$\mathbf{Q}$ structure, modulating the spins in the orthogonal direction, would be energetically degenerate in the extended Heisenberg model (including biquadratic and cyclic four-spin terms) but is disfavored by the 3-site 4-spin term. Our calculations suggest that the size of this term can be as large (or even exceed) the well known four-spin interactions and that this finding is not limited to the Fe/Rh system.

[1] A. Al-Zubi et al., phys. stat. sol. (b) **248**, 2242 (2011).
[2] A. Krönlein et al., submitted (2017).

O 98.13 Thu 18:15 MA 042

Tuning the spin-related transport properties of FePc on Au(111) through single-molecule chemistry — •Ruoning Li and Yongfeng Wang — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing, China

Tuning the spin-dependent transport through molecules is of fundamental importance in single-molecule spintronics. Here, the transport properties of iron phthalocyanine (FePc) on Au(111) was investigated by a combination of scanning tunneling microscopy and density functional theory (DFT) calculations. In the high-resolution STS spectrum of FePc measured at 0.5 K, the Kondo resonance was observed. After removing its eight outermost hydrogen atoms, the spectroscopic feature changed to a double-step structure, which reflected a transition of molecular spin states. The DFT calculations revealed that the coupling between Fe and Au(111) got much weaker after cutting the hydrogen atoms. This explained the changing of the spin-related transport FePc on Au(111).

O 99: 2D materials beyond graphene: TMDCs, silicene and relatives IV

Time: Thursday 15:00–17:45 Location: MA 043

O 99.1 Thu 15:00 MA 043

Ultrafast Dynamics of Single Layer TaS_2 — •Federico Andreatta[1], Antonija G. Čabo[1], Deepnarayan Biswas[2], Charlotte E. Sanders[1], Marco Bianchi[1], Cephise Cacho[3], Alfred Jones[3], Richard T. Chapman[3], Emma Springate[3], Phil D. C. King[2], Jill A. Miwa[1], Søren Ulstrup[1], and Philip Hofmann[1] — [1]Aarhus University, DK — [2]University of St. Andrews, UK — [3]CLF, STFC Rutherford Appleton Laboratory, UK

Metallic transition metal dichalocogenides, synthesized on single crystal metal substrates, have been recently explored down to the single layer limit[1,2]. Here, we synthesize metallic single layer tantalum disulphide (TaS_2) on graphene on silicon carbide to create a model two-dimensional van der Waals heterostructure. Not only do we probe the static electronic properties of the single layer TaS_2 but also the nonequilibrium carrier dynamics by means of time-and-angle resolved photoemission spectroscopy[3]. We present a novel way to fit the spectral function of the band dispersion at the Fermi level so that the band renormalization is tracked on a femtosecond time-scale.

[1] M. Dendzik, et al. Physical Review B, 92(24), 2015. [2] C. E. Sanders, et al. Physical Review B, 94(8), 2016. [3] S. Ulstrup, et al. ACS Nano, 10(6):6315-6322, 2016.

O 99.2 Thu 15:15 MA 043

Realistic Description of Competing Interactions in Metallic TMDCs — Ebad Kamil[1], Gunnar Schönhoff[1], Malte Rösner[1,2], •Jan Berges[1], and Tim Wehling[1] — [1]Institut für Theoretische Physik, Bremen Center for Computational Materials Science, Universität Bremen, Germany — [2]Department of Physics and Astronomy, University of Southern California, Los Angeles, USA

Two-dimensional transition metal dichalcogenides constitute a prominent showplace for competing many-body instabilities such as superconductivity [Frindt: PRL **28**, 299 (1972)], charge-density waves [Ugeda *et al.*: Nat. Phys. **12**, 92 (2016)] and magnetism [Ma *et al.*: ACS Nano **6**, 1695 (2012)]. In this study, we show that even though the observed phase diagrams are complex, the underlying mechanisms are captured by a compact unifying theoretical framework. We apply the constrained random-phase approximation (cRPA) [Aryasetiawan *et al.*: PRB **74**, 125106 (2006)] and constrained density-functional perturbation theory (cDFPT) [Nomura, Arita: PRB **92**, 245108 (2015)] to the metallic monolayers H-MX_2 with $M \in \{\mathrm{V}, \mathrm{Nb}, \mathrm{Ta}\}$ and $X \in \{\mathrm{S}, \mathrm{Se}\}$ and summarize the material specifics with a small number of representative Coulomb and electron-phonon interaction parameters. Both cRPA and cDFPT imply a separation of the electrons into a correlated subspace, here an isolated metallic band, and the rest. We find that all relevant physics emerge from interactions within this subspace. Beyond that, the materials can be well described by very similar tight-binding and mass-spring models.

O 99.3 Thu 15:30 MA 043

Direct determination of monolayer MoS2 and WSe2 exciton binding energies on insulating and metallic substrates — •Soohyung Park[1,2], Niklas Mutz[1], Thorsten Schultz[1], Ali Han[3,4], Areej Areej[3,4], Lain-Jong Li[3,4], Emil J. W. List-Kratochvil[1], Patrick Amsalem[1], and Norbert Koch[1,2] — [1]Humboldt-Universität, Berlin, Germany — [2]Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany — [3]Research Center for Applied Sciences, Taipei, Taiwan — [4]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Two-dimensional transition-metal dichalcogenides (2D TMDCs) are attractive candidates for next-generation optoelectronic devices due to their unique electronic and optical properties. To employ 2D TMDCs in optoelectronic devices, understanding the fundamental physical properties is necessary. In this regard, one key parameter is the exciton binding energy. It is the energy difference between the lowest-energy optical absorption (optical gap) and the charge transport energy gap (transport gap). In this contribution, we will present an experimental study combining angle-resolved direct and inverse photoelectron spectroscopy in order to measure the transport gap, and reflectance measurements for a determination of the optical gap. In this manner we are able to determine the exciton binding energy for two common 2D TMDCs, MoS2 and WSe2, on insulator and metal substrates. In addition, we will show that the dielectric environment of 2D TMDCs strongly impacts the transport gap while the optical gap is barely affected, indicating large exciton binding energy change.

O 99.4 Thu 15:45 MA 043

One-dimensional states confined within mirror twin boundaries in MoS_2 — •Wouter Jolie[1,2], Clifford Murray[1], Philipp Weiss[3], Joshua Hall[1], Fabian Portner[3], Nicolae

Atodiresei[4], Arkady Krasheninnikov[5], Hannu-Pekka Komsa[6], Achim Rosch[3], Carsten Busse[1,2,7], and Thomas Michely[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [3]Institute for Theoretical Physics, University of Cologne, Germany — [4]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [5]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [6]Department of Applied Physics, Aalto University, Finland — [7]Department Physik, Universität Siegen, Germany

We investigate epitaxial, single-layer MoS$_2$ on graphene on Ir(111) with scanning tunneling microscopy and spectroscopy (STM/STS). We find a large bandgap of 2.50 ± 0.05 eV in MoS$_2$ showing that it is well decoupled from the substrate. The MoS$_2$ islands feature two types of long, straight, highly symmetric mirror twin boundaries. Along these we measure a small bandgap of the order of 0.1 eV, together with periodic beatings in the local density of states. Using ab initio calculations, these features are traced back to one-dimensional metallic twin boundary states. We will critically discuss the contributions of confinement (finite wire length), Peierls instability (charge density wave formation) and spin-charge separation to explain the observed features.

O 99.5 Thu 16:00 MA 043

Coupling mechanisms of transition metal dichalcogenides to plasmonic gold nanoparticle arrays — •Jonas Kiemle[1,2], Sandra Diefenbach[1,2], Sebastian Funke[3], Peter Thiesen[3], Ursula Wurstbauer[1,2], and Alexander W. Holleitner[1,2] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany — [3]Accurion GmbH, Stresemannstr. 30, 87079 Göttingen, Germany

We reveal the manifold interaction mechanisms between monolayers of MoS$_2$ and single layers of plasmon-active gold nanoparticles. The MoS$_2$ shows a ten- to twenty-fold enhanced photoluminescence when it is decorated with the gold nanoparticles. Surprisingly, we detect this enhancement also for excitation energies, which are not resonant to the surface plasmon polaritons of the nanoparticles. Complementary Kelvin probe force measurements indicate a lowering of the work function, when the MoS$_2$ is decorated with the gold nanoparticles. This is in agreement with a reduced band gap for the decorated MoS$_2$ as determined from absorbance measurements. We furthermore demonstrate a dielectric coupling between the two layers by spectroscopic imaging ellipsometry as well as Raman spectroscopy. Combining the various results, we discuss the enhanced photoluminescence in terms of a modified emission pattern of the radiative dipole in the MoS$_2$ monolayers at the presence of the gold nanoparticles.

O 99.6 Thu 16:15 MA 043

Electronic characterization of the coexisting charge density wave and superconductivity in single-layer NbSe2 at T = 1 K — •Carmen Rubio-Verdú[1], Deung-Jang Choi[1], Hyejin Ryu[2], Sung-Kwan Mo[2], Zhi-Xun Shen[3,4], José Ignacio Pascual[1,5], and Miguel M. Ugeda[1,5] — [1]CIC nanoGUNE, San Sebastián, Spain — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, USA — [3]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, California, USA — [4]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University, Stanford, California, USA — [5]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Single-layer NbSe2 has been studied by means of low-temperature STM/STS. Our STS measurements reveal the coexistence of CDW order and 2D superconductivity at T = 1 K. We spatially mapped the conductivity of the NbSe2 layer at T = 1 K with atomic resolution to reveal strong oscillations of the depth and width of the superconducting gap with well-defined wavelength of 7 Å, coincident with that of the quasiparticle interference (QPI) patterns visible at the Fermi energy. This phenomenon is accompanied by intriguing spatial dynamics of the QPI patterns for energies within the SC gap.

15 min. break

O 99.7 Thu 16:45 MA 043

Characterization of Collective Ground States in Single-layer NbSe2 — •Miguel M. Ugeda[1,2,3], Aaron J. Bradley[1], Yi Zhang[4], Seita Onishi[1], Claudia Ojeda-Aristizabal[1], Hyejin Ryu[4], Alexander Riss[1], Sung-Kwan Mo[4], Dunghai Lee[1], Alex Zettl[1,5], Zahid Hussain[4], Zhi-Xun Shen[6,7], and Michael F. Crommie[1,5] — [1]Department of Physics, University of California at Berkeley, Berkeley, California, USA. — [2]CIC nanoGUNE, Donostia-San Sebastian, Spain. — [3]Ikerbasque, Basque Foundation for Science, Bilbao, Spain. — [4]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, USA. — [5]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, USA. — [6]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, California, USA. — [7]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University, Stanford, California, USA.

In bulk NbSe2 a CDW sets in at 33K and superconductivity at 7.2K and their microscopic formation mechanisms remain controversial. In this talk I will present the electronic characterization of a single layer of NbSe2 by means of STM/STS, ARPES, and transport measurements (1,2). I will show that 3x3 CDW order in NbSe2 remains intact in 2D. Superconductivity also still remains in 2D, but its onset temperature is depressed to 1.9K. Our STS measurements reveal a CDW gap of 4 meV at EF, which is accessible due to the removal of bands crossing EF for a monolayer. [1] Ugeda, Nature Physics 12, 92 (2016). [2]Onishi, PSS B 253, 2396 (2016).

O 99.8 Thu 17:00 MA 043

Electronic structure of single layer 1T-NbSe$_2$: interplay of lattice distortions, non-local exchange and Mott Hubbard correlations — •Ebad Kamil, Jan Berges, Gunnar Schönhoff, Malte Schüler, and Tim Wehling — Institut für Theoretische Physik, Universität Bremen, Bremen, Germany.

Transition metal dichalcogenides (TMDCs) often occur in two different crystal phases with octahedral (1T) and trigonal prismatic (2H) symmetry. For NbSe$_2$, the 2H phase has been known to be the most stable and easier to synthesize polymorph. However, recently 1T-NbSe$_2$ in the monolayer limit was synthesized epitaxially on a bilayer graphene and was suggested to be a Mott insulator [Yuki Nakata et al. NPG Asia Materials (2016) 8, e321] with $\sqrt{13} \times \sqrt{13}$ periodic density modulation. We perform ab-initio calculations to understand the emergence of an insulating behavior and charge density wave (CDW) in the monolayer 1T-NbSe$_2$, which otherwise is predicted to be a metal in DFT and GW calculations. We provide an estimate for the local and non-local screened Coulomb interaction within the ab-initio formalism and present the findings of LDA+DMFT simulations that suggest the possibility of opening of a Mott insulating gap in the CDW phase.

O 99.9 Thu 17:15 MA 043

Two-photon photoemission spectroscopy of the Dirac cone of a stanene-like Sn/Au(111) surface reconstruction — •M. Düvel[1], M. Maniraj[2], B. Stadtmüller[2,3], D. Jungkenn[2], M. Keunecke[1], S. Emmerich[2,3], D. Schmitt[1], W. Shi[4,5], L. Lyu[2], J. Stöckl[2], J. Kollamana[2], Z. Wei[2], A. Jurenkow[2], S. Jakobs[2], B. Yan[4], D. Steil[1], S. Steil[1], M. Cinchetti[6], M. Aeschlimann[2], and S. Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern — [3]Graduate School of Excellence Materials Science in Mainz — [4]MPI for Chemical Physics of Solids — [5]School of Physical Science and Technology, ShanghaiTech University — [6]Experimentelle Physik VI, Technische Universität Dortmund

Stanene, the graphene analog of Sn, was recently predicted and has subsequently motivated intense research on the realization of Sn-based ultrathin materials. Using photoelectron spectroscopy, we recently found a superstructure of Sn on Au(111) that reveals a Dirac-like band centered at the Γ-point with anti-parallel spin polarization and a Fermi velocity of $v_F \approx 1 \cdot 10^6$ m/s [Maniraj et al., submitted (2017)]. Using angle-resolved two-photon photoemission spectroscopy, we now access the unoccupied part of the electronic structure of this stanene-like reconstruction. We are able to map the dispersion of the unoccupied part of the surface states and therewith confirm their massless Dirac-like nature. Moreover, we find a series of image potential states, which we analyze in order to determine the interfacial coupling between the stanene-like layer and the Au substrate.

O 99.10 Thu 17:30 MA 043

First-principles calculations on the electronic, magnetic, and optical properties of NiPS$_3$ — •Tae Yun Kim and Cheol-Hwan Park — Department of Physics, Seoul National University, Seoul 08826, Korea

Magnetic van der Waals layered materials of transition metal phosphorous trichalcogednides (TMPX$_3$) have attracted attention as candidates that can support two-dimensional magnetism [1]. Because of the presence of localized d electrons of transition metals, it is natural to expect that TMPX$_3$ compounds may show some interesting phenomena arising from correlation effects. A recent experimental study revealed that the magnetic structure significantly affects the optical properties of NiPS$_3$, one of TMPX$_3$ compounds that exhibits antiferromagnetic phase below the Neel temperature at 154 K [2]. In this contribution, we discuss the electronic, magnetic, and optical properties of NiPS$_3$ in light of the experimental results based on our first-principles calculations.

[1] J. Park, J. Phys. Condens. Matter 28, 301001 (2016). [2] S. Y. Kim, T. Y. Kim, L. J. Sandilands, S. Sinn, M.-C. Lee, J. Son, S. Lee, K.-Y. Choi, W. Kim, B.-G. Park, C. Jeon, H.-D. Kim, C.-H. Park, J.-G. Park, S. J. Moon, T. W. Noh, arXiv:1706.06259 (2017).

O 100: Nanostructures at surfaces: Dots, particles, clusters II

Time: Thursday 15:00–17:00 Location: MA 141

Invited Talk O 100.1 Thu 15:00 MA 141
Suitably functionalized molecules on surface: from self-assembly to chemical reactions — •Shi-Xia Liu[1], Jascha Repp[2], Ernst Meyer[3], and Silvio Decurtins[1] — [1]Department of Chemistry and Biochemistry, University Bern, Freiestrasse 3, CH-3012 Bern, Switzerland — [2]Fakultaet fuer Physik, Universitaet Regensburg, D-93040 Regensburg, Germany — [3]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

A significant progress in the fields of surface science and nanotechnology has mainly been facilitated by single-molecule characterization techniques such as atomic force microscopy (AFM) and scanning tunneling microscopy (STM). Since chemical structures of individual molecules were resolved by AFM via the functionalization of the tip, identification of individual molecules on surfaces in various contexts including charge distribution, self-assembled structures and in situ visualization of on-surface chemical reaction products, have been highly motivated. This presentation puts emphasis on self-assembly and on-surface chemical reactions as well as electronic structures of appropriately functionalized molecules on surfaces.

O 100.2 Thu 15:30 MA 141
Studying Copper Growth on Zinc Oxide Utilizing a Neural Network Potential — •Martín Leandro Paleico and Jörg Behler — Universität Göttingen, Theoretische Chemie, Tammannstr. 6, 37077 Göttingen, Germany

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

The current work focuses on the initial results for the ternary copper-zinc oxide system. Specifically, we investigate the growth of copper clusters and films on zinc oxide surfaces using basin hopping Monte Carlo simulations, utilizing a NNP to provide the required energies and forces.

O 100.3 Thu 15:45 MA 141
Highly reproducible surface-enhanced Raman scattering substrate for detection of phenolic pollutants — •Zhiqiang Zeng[1,2], Rui Xu[1], and Yong Lei[1] — [1]Technische Universität Ilmenau, 98693, Ilmenau, Germany. — [2]South China Normal University, 510006,Guangzhou, China.

The ordering degree of nanostructures is the key to determining the uniformity of surface enhanced Raman scattering (SERS). However, fabrication of large-area ordered nanostructures remains a challenge, especially with the ultrahigh-density. Here, we report a fabrication of large-area ultrahigh-density ordered Ag@Al2O3/Ag core-shell nanosphere (NS) arrays with tunable nanostructures. The ultrahigh-density ordered NS arrays over a large-area capability (diameter >4.0 cm) enable the uniform SERS signals with the relative standard deviation of less than 5%. The as-fabricated highly reproducible SERS substrate can be applied to detect trace phenolic pollutants in water. This work does not only provide a new route for synthesizing the ultrahigh-density ordered nanostructures, but also create a new class of SERS substrates with high sensitivity and excellent reproducibility.

O 100.4 Thu 16:00 MA 141
Probing water in confinement: a FT-RAIRS study of D2O nano clusters on a graphene-iridium moiré superstructure — •Robert Taube[1,2], Heshmat Noei[1], Marcus Creutzburg[1,2], and Andreas Stierle[1,2] — [1]DESY NanoLab, Deutsches Elektronensynchrotron (DESY), Hamburg, Germany — [2]Institute of Nanostructure- and Solid State Physics, University of Hamburg, Germany

Confined water is highly interesting due to its unique properties regarding the molecular arrangement, electronic structure and the interaction with its neighboring environment. In this work, periodically arranged D2O nano droplets of about 1 nm size were generated on top of a graphene-iridium moiré superstructure and probed by a state-of-the-art Fourier transformation reflection absorption infrared spectrometer under UHV at 117 K. The infrared bands of the heavy water clusters differ significantly from those observed for amorphous solid or crystalline phases, showing a characteristic gap at 2500 cm-1 between two stretching bands. Furthermore, two features of dangling deuterium atoms originating from undercoordinated water molecules are present in the infrared spectrum. One of these features is located at noticeable lower wavenumbers than reported thus far, which is presumably the result of a rearrangement effect triggered by the coalescence of the droplets. The other feature originates from threefold coordinated water molecules at the surface of the water clusters and the film.

O 100.5 Thu 16:15 MA 141
General geometry DLVO model for particle deposition on patterned surfaces — •Joakim Löfgren, Johnas Eklöf, Kasper Moth-Poulsen, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

Molecular electronics holds the key to the continued miniaturization of transistors and diodes, and thus provides a pathway to next-generation electronics. In this context, the deposition of nanoparticles onto surfaces with pre-patterned features is currently being investigated as an efficient means for assembling circuits. Here, predictive modeling of the deposition process would provide an invaluable tool in designing optimized manufacturing protocols. Deposition problems are typically studied within the confines of DLVO theory, where interaction energies are given by analytical expressions but the geometry of the interacting entities is restricted to simple shapes such as spherical particles or flat surfaces, which renders them unsuitable for describing the deposition on patterned surfaces.

In this work we seek to remedy this situation by combining a general-geometry extension of DLVO theory with a random sequential adsorption algorithm to model the deposition onto pre-patterned surfaces. Finite-size effects are taken into account by modeling the geometry of the surface as a collection of virtual particles that interact with the deposited particle. The interaction potentials are based on analytical DLVO expressions and are fitted to reproduce the proper limiting forms. Using this approach we are able to predict optimal surface patterns for capturing particles in various pre-defined geometries.

O 100.6 Thu 16:30 MA 141
STM investigation of cluster-molecule hybrid systems deposited on the Si(111)$\sqrt{3}\times\sqrt{3}$ R30°-B surface — •Tim Amrhein[1], Martin Franz[1], Andre Knecht[2], Andrea Merli[2], Carl Frederic Ussling[2], Thomas Möller[2], and Mario Dähne[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik — [2]Technische Universität Berlin, Institut für Optik und Atomare Physik

Porphyrin based cluster-molecule hybrid systems may find application in constructing two-dimensional cluster arrays formed on a porphyrin template as well as give rise to new materials with tailored optical or electronic properties.

Here the cluster-molecule hybrid system Cu$_3$(Cu(OEP)) was prepared by combining Cu(II)Octaethylporphyrin with Cu$_3^+$-clusters in the gas phase, followed by a characterisation using mass spectroscopy and optical excitation. For further investigations of the atomic structure and electronic properties using STM, they were deposited onto a Si(111)$\sqrt{3}\times\sqrt{3}$ R30°-B surface, which was used because of its unique property of being passivated and semiconducting at the same time. To acquire the soft landing regime it was necessary to alter the kinetic energy of the positivly charged hybrids by applying an adjustable electric field. For the transport from the hybrid source to the STM a newly commissioned portable UHV-suitcase was used to preserve the UHV-conditions. First STM results of structures found on the surface will be presented.

This work was supported by the DFG through FOR 1282 projects D and G.

O 100.7 Thu 16:45 MA 141

Characterization of Soot Particles by Helium Ion Microscopy — •André Beyer[1], Daniel Emmrich[1], Maurin Salamanca[2], Lena Ruwe[2], Henning Vieker[1], Katharina Kohse-Höinghaus[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems and Surfaces, Bielefeld University, 33615 Bielefeld, Germany — [2]Department of Chemistry, Bielefeld University, 33615 Bielefeld, Germany

Complementary techniques for the characterization of soot particles are needed to gain insight into their formation processes. In this contribution, we focus on Helium Ion Microscopy (HIM) which allows high contrast imaging of soot particles with sizes down to 2 nm. Soot formation was realized with well-defined model flames from different fuel compositions. The particles were sampled on silicon substrates at different positons within the flame which allows choosing the particles degree of maturity. Large numbers of particles were recorded with a single HIM image in a relatively short time. A number of such images were combined to obtain meaningful particle size distributions. In addition, the following geometric properties of soot particles were evaluated: sphericity, circularity, and fractal dimension. Comparison with other experimental techniques as well as theoretical model calculations demonstrate the strength of HIM as a soot characterization method [1-3].

[1] M. Schenk et al., ChemPhysChem 14 (2013) 3248.
[2] M. Schenk et al., Proc Combust Inst 35 (2015) 1879.
[3] C. Betrancourt et al., Aerosol Sci. Technol. 51 (2017) 916.

O 101: Focus Session: Structural Dynamics in Nanoscale Materials, Probed by Ultrafast Electron Pulses II

Time: Thursday 15:00–17:30 Location: HE 101

Invited Talk O 101.1 Thu 15:00 HE 101

Ultrafast Structural Dynamics in Organic Molecular Solids — •Heinrich Schwoerer — Max Planck Institut für Struktur und Dynamik der Materie, Hamburg, Germany

Research on functional organic materials is driven by their chemically tunable optoelectronic properties which have led to many commercial applications, notably including molecular semiconductors such as organic light emitting diodes (OLEDs) and organic photodetectors. Comprised of molecules with strong internal covalent bonds which determine the optical characteristics, the macroscopic electronic properties of such crystals are predominantly set by the structural order, which is in turn determined by weak intermolecular forces. This hierarchy of forces opens two approaches for structural dynamics investigations: making use of the crystalline phase of organic molecules to study photo-induced chemical reactions (within the limitations of the confinement), and, looking beyond the unit cell, observing the ultrafast microscopic dynamics responsible for photo-induced macroscopic phase transitions in the entire organic crystal. We will introduce intriguing properties of organic molecular crystals and present recent examples of either of these approaches.

Invited Talk O 101.2 Thu 15:30 HE 101

Ultrafast Electronic Band Gap Control and Self-Protection from a Photoinduced Phase Transition in an Excitonic Insulator — •Julia Stähler — Dept. of Physical Chemistry, Fritz Haber Institute Berlin, Faradayweg 4-6, 14195 Berlin

Ta$_2$NiSe$_5$ is proposed to support an excitonic insulator phase below T_C = 328 K combined with a structural change. The former occurs in small gap semiconductors with strong electron-hole interaction where excitons form spontaneously and condense into a new insulating ground state. We study the ultrafast electron and lattice dynamics of Ta$_2$NiSe$_5$ by means of time- and angle-resolved photoemission spectroscopy (trARPES) and time-resolved coherent optical phonon spectroscopy. We find that the low temperature structural phase persists even for high excitation densities and the photoinduced structural phase transition is hindered by absorption saturation of excitation pulses at a fluence of $F_\mathrm{C} = 0.2$ mJ cm^2. We also show that the electronic band gap can be optically controlled by tuning the excitation density. Below F_C, the band gap shrinks transiently due to photoenhanced screening of the Coulomb interaction. However, above F_C, the band gap transiently widens at the Gamma point and recovers to its equilibrium value after 1.5 ps. Hartree-Fock calculations reveal that the band gap widening is due to photoenhancement of the exciton condensate density, persisting until interband carrier relaxation occurs. These results demonstrate the possibility to manipulate exciton condensates with light and gain ultrafast band gap control.

15 min. break

O 101.3 Thu 16:15 HE 101

Optically excited structural transition in atomic wires on surfaces at the quantum limit: a femtosecond ultrafast surface electron diffraction study — Tim Frigge[1], Bernd Hafke[1], Tobias Witte[1], Boris Krenzer[1], Manuel Ligges[1], Uwe Bovensiepen[1], Stefan Wippermann[2], Wolf Gero Schmidt[2], and •Michael Horn-von Hoegen[1] — [1]Fakultät für Physik und CENIDE, Uni Duisburg-Essen, Germany — [2]Theoretische Materialphysik, Uni Paderborn, Germany

The Indium induced (4x1) reconstruction on Si(111) is the prototype for 1D atomic wires at surfaces. At 130 K a metal-insulator transition to the (8x2) ground state takes place. A Peierls-like distortion causes periodicity doubling, opening of a band gap, and formation of a CDW. The non-equilibrium structural dynamics is studied by ultrafast RHEED with a fs-laser system in pump probe setup at temporal resolution better than 300 fs. Upon photo excitation the (8x2) ground state is driven in 350 fs to the (4x1) excited state as observed through the transient spot intensity changes. The transition is described in an accelerated displacive excitation scenario which relies on transient changes in the potential energy surface. The strong coupling between substrate and adsorbate is responsible for the sub-picosecond structural response by dephasing and damping the characteristic phonons in 1/4th of their oscillation period. Transient heating of the In atoms from 30 K to 80 K occurs delayed on a time scale of 2.2 ps. Thus the phase transition is driven by electronic entropy and not thermally.

O 101.4 Thu 16:30 HE 101

Phase-ordering kinetics of charge density waves mapped by ultrafast LEED — •Simon Vogelgesang[1], Gero Storeck[1], Jan Gerrit Horstmann[1], Theo Diekmann[1], Murat Sivis[1], Sebastian Schramm[1], Kai Rossnagel[2], Sascha Schäfer[1], and Claus Ropers[1] — [1]IV. Physical Institute - Solids and Nanostructures, University of Göttingen, Germany — [2]Institute for Experimental and Applied Physics, University of Kiel, Germany

Recently, ultrafast low-energy electron diffraction was developed for the investigation of structural dynamics in thin films in a transmission geometry [1]. In order to extend this approach to back-scattering diffraction for the analysis of surface dynamics, we employ miniaturized laser-driven electron sources featuring nanometric metal tip photocathodes [2]. Here, we investigate dynamics of charge density wave (CDW) phases at the surface of the quasi-two-dimensional material 1T-TaS$_2$ [3]. Specifically, we trace the laser-induced transition from the room-temperature nearly-commensurate (NC) to the high temperature incommensurate (IC) CDW phase. Performing a thorough spot-profile analysis, we identify a coarsening behavior in the newly created IC phase exhibiting significant CDW disorder. This growth of the IC CDW coherence length is attributed to the annihilation of dislocation-type topological defects, as corroborated by numerical simulations in a Ginzburg-Landau approach.

[1] M. Gulde et al., Science 345, 200 (2014). [2] G. Storeck et al., Structural Dynamics 4, 044024 (2017). [3] S. Vogelgesang et al., Nature Physics (2017), advance online publication, doi:10.1038/nphys4309.

O 101.5 Thu 16:45 HE 101

Ultrafast structural dynamics of transition metal dichalcogenide heterostructures — •Daniela Zahn, Thomas Vasileiadis, Lutz Waldecker, and Ralph Ernstorfer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Vertical heterostructures of two-dimensional crystals offer intriguing new perspectives for the fabrication of novel nanodevices [1]. Since all devices are operated in non-equilibrium conditions, interactions between the different degrees of freedom play an important role in their functionality. These interactions can be studied using femtosecond pump-probe techniques. In particular, femtosecond electron diffraction allows to directly observe the structural response to photoexcitation [2]. Electron-phonon and phonon-phonon coupling as well as electronic and vibrational coupling across interfaces can be studied.

We focus on heterostructures with staggered (=type II) band alignment. This particular band alignment leads to photo-induced charge separation across the interface and is therefore interesting for many applications, e.g. photovoltaic devices. We present a study on multilayer WSe_2/WS_2 heterostructures using two different excitation wavelengths. Different dynamics are observed, suggesting that the interfacial carrier transfer depends on the initial hot carrier distribution in k-space.

[1] A. Geim, I.V. Grigorieva, Nature 499, 419-425 (2013).

[2] L. Waldecker, R. Bertoni, R. Ernstorfer, JAP 117, 044903 (2015).

O 101.6 Thu 17:00 HE 101

Laser control of ultrafast nonthermal melting in silicon. — •Tobias Zier, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Femtosecond-laser pulses can induce structural phenomena, like, solid-to-solid phase transitions and ultrafast melting in crystalline structures. The main reason for the appearence of such effects is the ultrafast modification of the bonding properties in the induced nonthermal state consisting of extremely hot electrons and nearly not effected cold ions. Although melting is a stochastic process in thermodynamical equilibrium, we show that in the laser excited nonthermal case some coherences are preserved or created. Moreover, by performing ab initio molecular dynamics simulations of the excitation of silicon by a series of laser pulses we demonstrate that it is possible to control nonthermal melting by light. Analyzing the energy flow in quasimomentum space, we found that the ultrafast disordering atomic motion can be stopped and redirected depending on the delay between the pulses. Essential for the controlling mechanism is the appearance of an intermediate state in the excitation process that shows dominantly thermal phonon squeezing.

O 101.7 Thu 17:15 HE 101

Ab-initio calculation of electron impact ionization cross sections for atoms in exotic electron configurations — •John Bekx[1,2], Sang-Kil Son[1], Robin Santra[1,2], and Beata Ziaja[1,3] — [1]DESY, Hamburg, Germany — [2]University of Hamburg, Hamburg, Germany — [3]INP, Krakow, Poland

Coherent diffraction imaging uses intense femtosecond pulses of hard X-rays. When such pulses interact with the imaged sample, photoelectrons from atomic inner shells are ionized. In light elements, the core holes formed relax predominantly through Auger decay, whose characteristic lifetime is usually between 1 and 10 fs. During this time interval, due to the presence of many energetic electrons excited by X-rays, the ions with core holes may also undergo impact ionization. In this study, we investigate the impact ionization cross sections of ions with such exotic electron configurations and compare them to those of ground state atoms and ions. For calculating the doubly differential cross section, both energy- and angle-resolved, we extend the ab-initio toolkit XATOM [1]. We use the Born approximation for the impact electron, and apply the Hartree-Fock-Slater model for the description of the complex many-electron system under consideration. Our predictions have important implications for understanding radiation damage in X-ray free-electron laser experiments. We also expect applications in the area of electron diffraction, where similar bound-electron configurations could arise.

[1] Z. Jurek, et al., J. Appl. Crystallogr. **49**, 1048-1056 (2016).

O 102: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France Paul R. Kent, Oak Ridge National Laboratory, USA Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Thursday 15:00–17:45 Location: HL 001

Invited Talk O 102.1 Thu 15:00 HL 001

Recent developments in FCIQMC: real-time propagation and improved convergence with walker number — •Ali Alavi — Max Planck Institute for Solid State Research, Stuttgart, Germany

The Full Configuration Interaction QMC method samples Slater determinants using an imaginary-time propagation of walkers, and can yield essentially exact ground- and excited states energies and wavefunctions for Fermionic systems. Recently we have extended this methodology to real-time propagation, enabling the calculation of spectral functions along the real-frequency axis. This method will be described in the talk, together with representative examples from molecular and lattice models. We will also describe a second development in the FCIQMC methodology which substantially improves the rate of convergence of the ground-state technique with respect to the number of walkers. With the new method, we can compute essentially the exact ground state energy of the benzene molecule, correlating 30 electrons (the entire valence) in the full set of 108 orbitals of a VDZ basis. Perspectives of the new methods will be discussed.

O 102.2 Thu 15:30 HL 001

Quasi-Continuous LDA+DMFT calculations for SrVO3. — •Evan Sheridan, Christopher Rhodes, Evgeny Plekhanov, and Cedric Weber — King's College London, Theory and Simulation of Condensed Matter (TSCM), The Strand, London, United Kingdom.

The Dynamical Mean Field Theory (DMFT) is an extremely powerful tool in the treatment of strongly correlated electron systems and many DMFT calculations suffer from a computational bottleneck when it attempts to solve the Anderson Impurity Model (AIM).

Common among the early Anderson Impurity solvers was the Auxiliary Field Quantum Monte Carlo (AF-QMC) approach which relies on a discretisation of the imaginary time grid. AF-QMC solvers suffer from the notorious Suzuki-Trotter error,as a result of this , that has largely been ignored in recent years with the advent of Continuous Time-QMC (CT-QMC) solvers.

Here, we present a systematic study of how this issue can be overcome for realistic material properties using LDA+DMFT. We find that our quasi-continuous time method compares well to the state-of-the-art CT-QMC calculations for SrVO3, with the added advantage of linear scaling in temperature. The theoretical framework proposed is quite general and can be extended to cluster DMFT calculations.

O 102.3 Thu 15:45 HL 001

High temperature superconducting oxychlorides: a light element model for cuprates — •Matteo d'Astuto[1,2], Blair Lebert[2,3], Ikuya Yamada[4], and Masaki Azuma[5] — [1]Institut NEEL CNRS/UGA UPR2940 25 rue des Martyrs BP 166 38042 Grenoble cedex 9 FRANCE — [2]IMPMC, UMR7590 UPMC-Sorbonne Universités - CNRS, Paris, France — [3]Synchrotron SOLEIL, Gif-sur-Yvette, France — [4]Nanoscience and Nanotechnology Research Center (N2RC),

Osaka, Japan — [5]Materials and Structures Laboratory, TITech, Yokohama, Japan

The copper oxychloride cuprate $Ca_2CuO_2Cl_2$ (CCOC) system, with vacancy or Na doping on the Ca site, is unique among the high temperature superconducting cuprates (HTSCs) since it: lacks high Z atoms; has a simple I4/mmm 1-layer structure, typical of 214 (LSCO) cuprates, but which is stable at all doping and temperatures; and has a strong 2D character due to the replacement of apical oxygen with chlorine. It also shows a remarkable phase digram, with a superconducting T_C growing to the optimal doping without any minimum around 1/8 doping, despite the observation of charge modulations by near-field spectro-microscopy. Due to the reduced number of electrons, advanced calculations that incorporate correlation effects, such as quantum Monte Carlo are easier, but relatively little is known about CCOC (for a cuprate) from an experimental point of view. We are now filling this gap by a comprehensive experimental study covering the whole phase diagram, in particular of the (para)magnon and phonon dispersion..

O 102.4 Thu 16:00 HL 001

Antiferromagnetic correlations in the metallic strongly correlated transition metal oxide $LaNiO_3$ — •Hanjie Guo[1], Zhiwei Li[1], Li Zhao[1], Zhiwei Hu[1], Chunfu Chang[1], Changyang Kuo[1], Wolfgang Schmidt[2], Andrea Piovano[2], Tunwen Pi[3], Oleg Sobolev[4], Daniel Khomskii[1], Liu Hao Tjeng[1], and Alexander Komarek[1] — [1]MPI CPfS, Dresden, Germany — [2]ILL, Grenoble, France — [3]NSRRC, Taiwan — [4]FRMII, Munich, Germany

The material class of rare earth nickelates with high Ni^{3+} oxidation state is generating continued interest due to the occurrence of a metal-insulator transition with charge order and the appearance of non-collinear magnetic phases within this insulating regime. The recent theoretical prediction for superconductivity in $LaNiO_3$ thin films has also triggered intensive research efforts. $LaNiO_3$ seems to be the only rare earth nickelate that stays metallic and paramagnetic down to lowest temperatures. So far, centimetre-sized impurity-free single crystal growth has not been reported for the rare earth nickelates material class since elevated oxygen pressures are required for their synthesis. Here, we report on the successful growth of centimetre-sized $LaNiO_3$ single crystals by the floating zone technique at oxygen pressures of up to 150 bar. Our crystals are essentially free from Ni^{2+} impurities and exhibit metallic properties together with an unexpected but clear antiferromagnetic transition.

O 102.5 Thu 16:15 HL 001

First-principles quantum Monte Carlo study of correlated materials — •Huihuo Zheng — Argonne Leadership Computing Facility, Argonne National Laboratory, Lemont, USA

Strongly correlated electronic systems have become an important subject of condensed matter physics, because of many fascinating phenomena arising in these systems such as metal-insulator transition, high temperature superconductivity, etc. Accurate characterization of the electron-electron correlations in these systems from first principles is essential for us to understand how these phenomena emerge from microscopic interactions. I will present our efforts in modeling correlated materials using the first-principles quantum Monte Carlo (QMC) method by showing two representative *ab intio* studies (vanadium dioxide and graphene) and a density-matrix downfolding theory for constructing low energy effective models from *ab initio* simulations. Using QMC, we correctly characterized the electronic structure of vanadium dioxide and unveiled the electronic origin of the metal-insulator transition which has been a mystery for decades. For graphene, we computed the electron screening from σ bonding electrons and illustrated how the emergent physics from underlying Coulomb interactions results in the observed weakly correlated semimetal. On the other hand, the downfolding approach we developed provides a way to quantitatively identify important microscopic interactions relevant to the macroscopic physics.

O 102.6 Thu 16:30 HL 001

Reduced Density Matrix Theory for Coupled Fermion-Boson Systems — •Florian Buchholz[1], Iris Theophilou[1], Michael Ruggenthaler[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]MPSD, Hamburg, Germany — [2]CCQ, The Flatiron Institute, New York, United Sates — [3]Nano-bio Spectroscopy Group, San Sebastián, Spain

Reduced density matrix (RDM) theory proved to be successful in describing a wide range of many-body problems that are not easily accessible by the more common many-body perturbation theories or density functional theory. Especially as RDM theories are non-perturbative, they are advantageous in strong coupling scenarios.

However, RDM theory was to our knowledge never applied to systems with more than one active particle type. The focus of this talk is to analyze the possibilities and problems of an extension to coupled fermion-boson theories. Comparing a typical bilinear interaction term of the form $c_i^+ c_j (a_k^+ + a_k)$, where c^+/c and a^+/a indicate fermion and boson creation/annihilation operators, respectively and the fermionic 2-body interaction term $c_i^+ c_j^+ c_k c_l$, the former should have a considerably reduced definition space, which we hope to be exploitable. On the other hand, the bilinear interaction has a very different structure than the 2-body interaction and it is not clear at all, how to define a RDM that carries all information to compute experimental observables of a coupled fermion-boson system.

Specifically, I will illustrate some of the peculiarities of the fermion-boson interaction for simple model systems and present some ideas to deal with those.

O 102.7 Thu 16:45 HL 001

Critical temperatures as function of magnetic anisotropy in two-dimensional systems from first-principles calculations — •Daniele Torelli — Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

Recent observation of ferromagnetic out-of-plane order in monolayer CrI_3 highlights the importance of a microscopic understanding of anisotropy in ground state magnetic systems. Single-ion anisotropy accounts mainly for spin-orbit coupling interaction and, in particular for two-dimensional (2D) materials, it's crucial to escape the Mermin-Wagner theorem. Here we investigate the variation of critical temperatures as functions of anisotropy in Heisenberg model systems using Metropolis Monte Carlo simulations. Results for square, hexagonal and honeycomb lattices are compared with equivalent simulations in the Ising model, which is confirmed to represent the limit with infinite anisotropy. Based on a new developed computational 2D materials database, we predict a vast number of 2D structures with high critical temperatures. As testing system, relevant Heisenberg exchange couplings and magnetic anisotropy energy in CrI_3 monolayer are extracted from first principle calculations and energy mapping analysis, yielding to an estimation of Curie temperature in good agreement with experimental results.

O 102.8 Thu 17:00 HL 001

Oxygen vacancy-induced absorption of visible light in SrNbO3 — •Marcello Turtulici, Steffen Backes, and Silke Biermann — Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau, France

SrNbO3 has recently attracted attention as a bright red photocatalyst. Several, mutually contradicting, models have been proposed in the literature in order to explain the strong absorption in the visible spectrum, and no consensus even on the basic nature of the mechanism has been reached. In this work we investigate the optical properties of this material by means of state-of-the-art Density Functional Theory and many-body perturbation theory techniques. We evidence a high sensitivity of the optical properties on deviations from the ideal crystal structure. In particular, the optical properties should strongly depend on the presence of oxygen vacancies, which give rise to additional absorption channels in the visible frequency range. Most notably, the experimentally observed red color is likely due to transitions between orbitals of dominant Nb-eg character, which are enhanced by the strong hybridization of the quite extended 4d-states of Nb with oxygen p-states.

O 102.9 Thu 17:15 HL 001

Transient charge and energy flow in the wide-band limit — Fabio Covito, •Florian Eich, Riku Tuovinen, Michael Sentef, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Thanks to recent advances in ultra-fast pump-probe spectroscopies and nano-thermometry it is possible to study charge and energy flow at atomic time and length scales. In order to analyze the transient dynamics of nanoscale devices theoretically, the wide-band limit is a commonly used approximation. Here we investigate the applicability of the wide-band limit to the study of charge and heat transport through nanojunctions exposed to voltage biases and temperature gradients. We find that while this approximation faithfully describes the long-time steady-state charge and heat transport, it fails to characterize the short-time transient behavior of the junction. In particular, we find that the charge current flowing through the device shows a discontinuity when a temperature gradient is applied, while the energy flow is discontinuous when a voltage bias drives the dynamics and even diverges when the junction is exposed to both a temperature gradient and a voltage bias. We discuss this pathological behavior and propose two possible solutions.

O 102.10 Thu 17:30 HL 001

From DFT to Coupled Cluster Theory - Understanding Oxygen Activation on Coin Metal Nanoparticles — •Wilke Dononelli and Thorsten Klüner — Institut für Chemie, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

In this study we focus on one of the most fundamental catalytic model reactions, the oxidation of CO on a metal catalyst. We studied the activation of molecular oxygen via dissociation or direct reaction of CO and O_2 within density functional theory (DFT) and high level CCSD(T) calculations. Therefore we use Au_{13} and Au_{55} nanoparticles (NPs) and a periodic Au(321) surface as model systems and compare the catalytic activity of the gold substrates to Ag and Cu based, as well as bimetallic NP catalysts. Part of the DFT calculations were performed, using the well-established PBE functional as implemented in the Vienna ab initio simulation package (VASP). Hybrid and double hybrid DFT calculations on the NPs were performed in Gaussian09. CCSD(T) calculation were performed in Gaussian09 using conventional CCSD(T) for the M_{13} (M=Au,Ag,Cu) NPs and CCSD(T)/PBE in a QM/QM embedding scheme using the ONIOM approach for M_{55} NPs. For systems of 55 metal atoms PBE gives the same results as double hybrids or even CCSD(T). For smaller M_{13} NPs interaction energies differ between PBE and higher levels of theory, which might be explained by the molecule like character of these NPs.

O 103: Oxide and Insulator Surfaces: Structure, Epitaxy and Growth II

Time: Thursday 15:45–16:30 Location: MA 041

O 103.1 Thu 15:45 MA 041

Germania Ultrathin Films on Different Substrates — •Adrian L. Lewandowski[1], Philomena Schlexer[2], Christin Büchner[1], Hannah Burrall[3], Kristen M. Burson[3], Wolf-Dieter Schneider[1], Gianfranco Pacchioni[2], Markus Heyde[1], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesselschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Department of Materials Science, Università di Milano-Bicocca, Via R. Cozzi, 55, Milan, Italy — [3]Taylor Science Center, Hamilton College, 198 College Hill Road, Clinton, NY 13323, USA

New insights into the structural configuration of amorphous networks have been obtained after imaging ultrathin silica bilayer films with scanning tunneling microscopy (STM) [1]. In order to establish a general understanding of amorphous networks more structural characterization of glass-former materials, such as germanium oxide, must be done. Germania ultrathin films were grown on Ru(0001) and Pt(111) by physical vapor deposition and subsequent annealing in oxygen. The atomically flat films were characterized by combining intensity-voltage low energy electron diffraction and ab initio density functional theory analysis with high-resolution STM imaging. The film-substrate interaction plays a decisive role in the film structure. On Ru(0001) a crystalline monolayer film with domain boundaries is obtained. At higher coverage disordered phases are revealed. On Pt(111) many different phases can be identified: monolayers with different symmetry, disordered layers at higher coverage and zigzag-line phases.

[1] L. Lichtenstein et al., Angew. Chem. Int. Ed. 51, 404 (2012)

O 103.2 Thu 16:00 MA 041

High-resolution force mapping on CaF_2(111) at 5 K, 77 K, and 300 K in UHV — •Fabian A. Schlage[1], Matthias Temmen[1], Adam M. Sweetman[2], Philip J. Moriarty[2], Matt Watkins[3], Michael Reichling[1], and Philipp Rahe[1] — [1]Universität Osnabrück, Germany — [2]University of Nottingham, UK — [3]University of Lincoln, UK

Force maps measured on CaF_2 (111) allow a detailed analysis of the atomic contrast formation of frequency shift measurements in non-contact atomic force microscopy and especially enable a quantification of interaction forces acting at the different sample sites. 2D force maps taken at room, liquid nitrogen, and liquid helium temperatures are compared. We analyze in detail forces at the atomic scale derived from the frequency shift maps by deconvolution. With these data, we then develop an interpretation for atomic contrast formation beyond the available models that are mainly based on electrostatic interactions.

O 103.3 Thu 16:15 MA 041

The structure of a two dimensional silica 'zigzag' polymorph on Ruthenium — •David Kuhness[1], Hyun Jin Yang[1], Hagen Klemm[1], Mauricio Prieto[1], Xin Yu[1], Denis Usvyat[2], Martin Schütz[2], Dietrich Menzel[1], Shamil Shaikhudtinov[1], Thomas Schmidt[1], Markus Heyde[1], Joachim Sauer[2], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany

Ultrathin two dimensional silica films grown on metal substrates serve as a model system for the study of glass. Its detailed study at the atomic scale allows for insights into its atomic structure, its growth modes, transformations and the herein involved dynamics. We here present a new two dimensional silica polymorph grown on a Ru(0001) metal substrate with characteristic 'zigzag' line structure and rectangular unit cell. Based on scanning tunneling microscopy, low energy electron diffraction, infrared reflection absorption spectroscopy and x-ray photo-electron spectroscopy measurements on the one hand, and density functional theory calculations on the other, a structural model for the 'zigzag' polymorph is proposed. In comparison to established monolayer and bilayer silica, this 'zigzag' structure system has intermediate characteristics in terms of coupling to the substrate and stochiometry. The silica 'zigzag' phase is transformed upon reoxidation at higher annealing temperature into a SiO_2 silica bilayer film which is chemically decoupled from the substrate.

O 104: Oxides and Insulators: Adsorption I

Time: Thursday 16:45–18:15 Location: MA 041

O 104.1 Thu 16:45 MA 041

Bulk Defect Dependent Adsorption of Acetone on Rutile TiO_2(110) — •Jessica Kräuter and Katharina Al-Shamery — Carl von Ossietzky University of Oldenburg, Institute of Chemistry, D-29129 Oldenburg

In chemical industry acetone is produced by the cumene process using peroxides. As alternative to get rid of the explosive peroxides a heterogeneous catalyzed process on TiO_2 is considered. As first step the adsorption of acetone on rutile TiO_2(110) was studied. Recently, an influence of the temperature dependent mobility of bulk defects on the reductive coupling of benzaldehyde was concluded from own work.[1] In previous coverage dependent studies on acetone and coadsorbed molecular oxygen the occurrence of a diolate species has been identified with surface science methods on a medium reduced rutile single crystal at liquid nitrogen temperatures.[2,3] Here we present the influence of bulk defects from studies on temperature dependent adsorption of acetone coadsorbed with molecular oxygen and oxygen adatoms. On a more strongly reduced rutile(110) single crystal a diolate species can be observed even without oxygen coadsorption. Furthermore, in TPRS an additional surface species appeared from 235 to 274 K when coadsorbing acetone with oxygen which has not been reported before. A possible β hydroxy ketone formation was identified by polarization dependent IRRAS measurement. [1] P. M. Clawin, C. M. Friend, K. Al-Shamery, A European Journal, 2014, 90, 7665. [2] M. A. Henderson, J. Phys. Chem. B, 2008, 108, 18932. [3] N. G. Petrik, M. A. Henderson, G. A. Kimmel, J. Phys. Chem. C., 2015, 119, 12273.

O 104.2 Thu 17:00 MA 041

Covalent Anchoring and Interfacial Reactions of Adsorbed Porphyrins on TiO_2(110) — •Daniel Wechsler[1], Cynthia Fernández[2], Hans-Peter Steinrück[1], Ole Lytken[1], and Federico Williams[2] — [1]Chair of Physical Chemistry II, University Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany — [2]Department of Inorganic, Analytical and Physical Chemistry, University of Buenos Aires, Buenos Aires C1428EHA, Argentina

Understanding the bonding between organic molecules and metal-oxide surfaces plays an important role in many nanotechnology devices. Functional groups, like -COOH, can act as linkers to attach molecules to surfaces in a controlled manner. We have studied the adsorption and covalent anchoring of 5-monocarboxyphenyl-10,15,20-triphenylporphyrin (MCTPP) on TiO_2(110) with X-ray Photoelectron Spectroscopy. At elevated temperatures, the free-base porphyrin molecules metalate on the surface, forming what we expect to be titanyl (Ti=O) porphyrin. The reaction is strongly coverage-dependent with lower coverages metalating at lower temperatures, possible caused by flat-lying molecules at low coverages being in closer proximity to the surface. We also find the metalation of porphyrins exposed to Zn^{2+} ions in solution to depend on the porphyrin coverage on the TiO_2(110) surface, but the effect is less pronounced.

The project is supported by the DFG trough FOR 1878 (funCOS).

O 104.3 Thu 17:15 MA 041

Hydroxy Species on TiO_2-Rutile(110): *ab initio* Adsorption Studies — •Niklas Thoben and Thorsten Klüner — Carl von Ossietzky Universität, Oldenburg, Germany

Since the deposits of fossil fuels are limited and therefore will run out in the future, the search for renewable energies and fuels is an important topic of today's researching activities. A promising candidate is molecular hydrogen produced by photocatalytic water splitting, which can be used in fuel cells to generate CO_2-free power [1]. To find new photocatalysts and make them more efficient an exact understanding of the elementary steps of the water splitting mechanism is needed.

In this contribution, we address the adsorption of hydroxy species on the titania-rutile(110) surface, which is found to be a suitable photocatalyst [2]. The investigated hydroxy species play an essential role in proposed reaction mechanisms [3]. In the calculations done with the MOLCAS program package we use an embedded cluster approach to describe the rutile(110) surface and the CASSCF/CASPT2 methodology for a faithful description of the electronic configuration of the system.

[1] C. Acar, I. Dincer, G.F. Naterer, *Int. J. Energy. Res.* **2016**, 40, 1449-1473.

[2] A. Fujushima, K. Honda, *Nature* **1972**, 238, 37-38.

[3] V. Diesen, M. Jonsson, *J. Phys. Chem. C* **2014**, 118, 10083-10087.

O 104.4 Thu 17:30 MA 041

***Ab initio* Cluster Calculations on the Adsorption and Electronic Excitation of SO_2 on TiO_2-Rutile(110)** — •Luca Gerhards and Thorsten Klüner — Carl von Ossietzky Universität, Oldenburg, Germany

The production of sulfonic acids as precursors for several products such as detergents or pharmaceutical drugs is a vital process for today's society. An efficient way to synthesize these compounds can be conducted by the sulfoxidation of alkenes. The photocatalytic heterogeneous sulfoxidation on titanium dioxides seems to be a promising new and more energy efficient alternative to the industrially applied homogeneous reaction. Experimental investigations on the mechanism revealed that the adsorption of SO_2 and the excitation with visible light lead to a formation of a charge-transfer complex on the surface which seems to catalyze the subsequent chain reaction.[1] These results stand in contrast to the homogenous mechanism and need a deeper investigation. In this contribution, we examine the adsorption and electronic excitation of SO_2 on the ideal TiO_2-rutile(110) surface from a quantum chemical perspective. For this purpose, an embedded cluster model was constructed in order to faithfully describe the substrate-adsorbate interaction. Along these lines, post-HF and multireference methods like MP2 or CASSCF/NEVPT2 as implemented in the program package ORCA were used to calculate electronic excitations of the adsorbate.

[1] F. Parrino, A. Ramakrishnan, H. Kisch, *Angew. Chem. Int. Ed.*, **47**(37), p. 7107-7109, 2008.

O 104.5 Thu 17:45 MA 041

Adsorption of Water and Organic Molecules on Magnetite (111) — •Marcus Creutzburg[1,2], Heshmat Noei[1], Björn Arndt[1,2], Elin Grånäs[1], Gregor Feldbauer[3], Kai Sellschopp[3], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron (DESY) — [2]University of Hamburg — [3]Institute of Advanced Ceramics, Hamburg University of Technology

Magnetite (Fe_3O_4) is an important transition metal oxide with diverse applications in catalysis, data storage and biomedical imaging. In a recent study magnetite nanoparticles linked by oleic acid molecules show exceptional isotropic mechanical properties [1]. To get insight into the interaction of these nanoparticles with organic molecules it is crucial to study flat single crystal surfaces. In this contribution, we present results on the adsorption of water and organic molecules like formic acid and oleic acid on the magnetite (111) surface under UHV conditions obtained by infrared reflection absorption spectroscopy and X-ray photoelectron spectroscopy. These findings are complemented by scanning tunneling microscopy results and surface X-ray diffraction measurements.

[1] A. Dreyer *et al.*, Nature Materials **15**, 522-528 (2016)

O 104.6 Thu 18:00 MA 041

Binding of Isophorone to single Au atoms on MgO(001) and Au(111) — •Niklas Nilius[1], Thomas Meyer[1], Christian Stiehler[1], Karoliina Honkala[2], and Hannu Häkkinen[2] — [1]Institute of Physics, Carl von Ossietzky University, D-26111 Oldenburg, Germany — [2]Departments of Physics and Chemistry, Nanoscience Center, University of Jyväskylä, P.O. Box 35, FI-40014 Finland

Formation of various metal/organic complexes comprising isophorone (C9H14O) and Au ad-atoms and clusters has been observed on MgO thin films by STM. The aggregates are hold together by electrostatic forces between the hydroxyl groups of the enol-isophorone and negative excess charges residing on the ad-gold. The energetically favorable keto-tautomer, on the other hand, is unreactive towards gold. DFT calculations find a tautomerization barrier between the keto- and enol-form of 0.76 eV on the MgO surface. On Au(111), no tautomerization takes places and isophorone physisorbs in the form of magic clusters containing four, six or nine molecules. Our study demonstrates how tautomerization of an unreactive ketone can be triggered by the presence of low-coordinated and charged metal ad-atoms on an oxide surface.

O 105: Nanostructures at surfaces: 1D and 2D structures and networks III

Time: Thursday 17:15–18:15 Location: MA 141

O 105.1 Thu 17:15 MA 141

Electrochemical switching of π-expanded macrocycles observed by STM/STS — •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

Macrocyclic oligothiophenes and their π-extended derivatives have attracted attention for their potential applications in molecular electronics and as components in molecular devices [1]. Here we investigated self-assembled monolayers of four π-expanded oligothiophene macrocycles 8-mers at the interface between their octanoic acid solutions and highly oriented pyrolytic graphite (HOPG). STM height images showed hexagonal ordered 2D-networks with a small difference in unit cells. I–V characteristics confirmed the donor like character of the macrocycles, whose HOMO and LUMO position were consistent with TD-DFT calculations. Moreover, optical gaps determined from UV-Vis absorption and TD-DFT resulted in accordance with the effective gap measured by STS. Cyclic STS measurements showed the switching from the diastereomer *Z,Z*-8-mer to the *E,E*-8-mer form after formation of a most stable cationic species, which confirms voltammetry and chemical oxidation experiments. To the best of our knowledge, this result represents the first electrochemical switching experiment under standard STM conditions.

[1] M. Iyoda and H. Shimizu. *Chem. Soc. Rev.*, **44**(18): 6411-6424, 2015

O 105.2 Thu 17:30 MA 141

Crossover in the inelastic spectra of highly-conducting conjugated molecules — •Enrique Montes, Giuseppe Foti, and Héctor Vázquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Prague, Czech Republic

We use inelastic electron tunnelling spectroscopy (IETS) first-principles simulations [1] to identify and characterise the different vibrational modes of single conjugated molecules bonded to Au metal electrodes. The molecules are polyphenyls (with 1 to 4 benzene units) bonded to Au via highly conducting direct Au-C bonds. The short molecule shows near resonant elastic transmission, with a crossover to tunnelling for the longer backbones [2].

The calculated inelastic spectra exhibit dips for the short molecule, and peaks for the longer molecules, in the second derivative of the current. We first characterize the inelastic spectra in terms of IETS selection rules [3]. We then analyze the observed trends as a function of molecular length. In particular, we characterize the modes whose inelastic signal increases with the number of phenyl units, the modes where it decreases, and the modes where IETS dips change to peaks.

[1] T. Frederiksen, M. Paulsson, M. Brandbyge, and A.-P. Jauho. Phys. Rev. B 75, 205413 (2007).

[2] W. Chen, J. R. Widawsky, H. Vázquez, S. T. Schneebeli, M. S. Hybertsen, R. Breslow, and L. Venkataraman. J. Am. Chem. Soc. 133, 17160 (2011).

[3] M. Paulsson, T. Frederiksen, H. Ueba, N. Lorente, and M. Brandbyge. Phys. Rev. Lett. 100, 226604 (2008).

O 105.3 Thu 17:45 MA 141

Hierarchical nanostructures by combining block copolymer and nanosphere lithography — •Daniel Kool[1,2], Katharina Brassat[1,2], and Jörg K. N. Lindner[1,2] — [1]Paderborn University, Dept. of Physics, Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn, Germany

Block copolymer (BCP) lithography is a well-established technique for economical large-area surface structuring exploiting the microphase separation of a copolymer, here poly(styrene-b-methylmethacrylat) (PS-b-PMMA) BCP into self-assembled nanopatterns. Using a block length ratio of 70:30 we achieve perpendicular, 17 nm diameter PMMA cylinders hexagonally arranged in a PS-Matrix. After removing selectively the PMMA cylinders a pore density up to $9.5 \cdot 10^{10}$ cm^{-2} is achieved. SEM images are evaluated by a self-written Delaunay-triangulation based software. In order to guide the self-assembly process of nanopores, we prepattern the substrate surface using nanosphere lithography (NSL). To this end convective self-assembly of polystyrene nanospheres in a colloidal suspension in used to generate a hexagonally close packed array of spheres. Spheres are shrunk in an oxygen plasma and used as a shadow mask in a metal thin film deposition. After removal of the sphere mask a hexagonal array of open cylinders (antidots) in the metal film is achieved. We demonstrate that using these antidots as template for the BCP lithography allows for the site-selective creation of both nanopore arrays and concentric PS rings inside antidots.

O 105.4 Thu 18:00 MA 141

Antiaromaticity as p-doping of the aromatic electronic structure. — •Narendra Prabhakar Arasu and Héctor Vázquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10/112, Prague, Czech Republic

Hückel's rule states that cyclic and planar π-system is aromatic when it shares $4n + 2$ π-electrons and antiaromatic when it possesses 4n electrons. Electrochemical studies had predicted antiaromatic molecules to have excellent conducting properties [1,2] but their instability limited their study. Recently, the single molecule conductance of a genuinely antiaromatic molecule was measured for the first time [3].

In this talk, I will describe our study on the electronic structure and conductance of aromatic and antiaromatic molecular junctions using first-principle calculations. First, I will compare the conductance of an aromatic porphyrin backbone with that of a norcorrole antiaromatic unit. We found that the conductance of the antiaromatic molecule was much higher than that of the aromatic counterpart [3]. I will then generalize this analysis to a series of aromatic-antiaromatic pairs of molecules. From a quantitative analysis of the similarity in their electronic structure, antiaromaticity is found to correspond to p-doping of the aromatic electronic structure. We generalize this analysis to explain the higher conductance of quinones [2] and discuss the implications for single molecule transport.

[1] R. Breslow et al., J. Am. Chem. Soc, 95 (20), 6688 (1973). [2] R. Breslow et al., J. Phys.: Condens. Matter, 20, 374104 (2008). [3] S. Fujii et al., Nat. Commun, 8, 15984 (2017).

O 106: Annual Meeting of the Surface Science Division

Time: Thursday 19:00–19:30 Location: H 0105

Topics: Report of the Chairman; Presentation of the Gerhard Ertl Young Investigator Award; Elections; Miscellaneous

O 107: Post-Deadline Session

Time: Thursday 19:30–20:30 Location: H 0105

Contributed Post-Deadline Talks

O 108: Overview Talk: Shuyun Zhou

Time: Friday 9:30–10:15 Location: HE 101

Invited Talk O 108.1 Fri 9:30 HE 101

Electronic structure of two-dimensional materials revealed by angle-resolved photoemission spectroscopy (ARPES) and Nano-ARPES — •Shuyun Zhou — Tsinghua University, Beijing, China 100084

Transition metal dichalcogenides (TMDCs) are important for both their intriging physics and potential applications. Revealing the electronic and spin structure is critical for understanding the physical properties as well as exploring their potential appications. Here I will present our experimental investigations on the electronic structures of a few TMDCs using advanced electron spectroscopies, including angle-resolved photoemission spectroscopy, Nano-ARPES and spin-resolved ARPES.

O 109: Focus Session: Molecular Nanostructures on surfaces - New Concepts towards Complex Architectures VII

Organizers: Sabine Maier, FAU Erlangen-Nürnberg; Meike Stöhr, University of Groningen

(Synopsis provided with part I of this session)

Time: Friday 10:30–11:45 Location: MA 004

O 109.1 Fri 10:30 MA 004

Insight into the unit cell: Structure of picene thin films on Ag(100) revealed with complementary methods — •Tobias Huempfner, Martin Hafermann, Christian Udhardt, Felix Otto, Roman Forker, and Torsten Fritz — Friedrich Schiller University, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

We studied the molecular structure of one monolayer of picene on a Ag(100) surface. Low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) experiments show that the molecules arrange in a highly ordered manner exhibiting a point-on-line epitaxy with two differently arranged molecules per unit cell. Besides the structural investigations, we also studied the electronic properties via photoelectron spectroscopy. In particular, we recorded photoelectron momentum maps (PMMs) at different binding energies. PMMs based on molecular orbitals obtained from density functional theory (DFT) calculations of free molecules are simulated for a better understanding of the measured maps. Comparing measured and simulated PMMs allows further conclusions about the composition of the unit cell. The structural basis consists of two parallel molecules; one molecule lies face-on and the other is tilted by 45° around its long axis with respect to the surface normal.

O 109.2 Fri 10:45 MA 004

construction of sierpiński triangles up to the fifth order — Chao Li, Xue Zhang, Na Li, •Jiajia Yang, and Yongfeng Wang — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Self-similar fractal structures are crucial in science, mathematics, and aesthetics. Recently, a series of molecular defect-free fractals of Sierpiński Triangles (STs) have been constructed on surfaces. In those previous experiments, the highest order of STs is simply 4th due to the random formation of nucleation centers and the limitation of kinetic growth. The growth mechanism of STs was investigated by low-temperature scanning tunneling microscopy. Here, we used a templating method to guide the formation of nucleation centers and co-assembly method to overcome the kinetic-growth limitation and control the formation of STs. Owing to the templating effect of the reconstructed Au(100)-(hex) substrate, Fe atoms, 4,4”-dicyano-1,1’:3’,1”terphenyl (C3PC), and 1,3-bis(4-pyridyl)benzene (BPyB) molecules were used to build fractals. According to our experiments, the proper C3PC : BPyB ratio is need to obtain the 5th-order STs. When C3PC molecules dominate, it tends to form a 1D crystalline chain structure. With large rate of BPyB to C3PC, the surface structures are determined by BPyB molecules and only small STs are obtained. The new strategy may be applied to construct various Sierpiński triangles of higher orders.

O 109.3 Fri 11:00 MA 004

Oxygen-triggered electronic and structural decoupling at the PTCDA/Cu(100) interface — •Xiaosheng Yang[1,2], Simon Weiss[1,2], Ina Krieger[3], Timo Heepenstrick[3], Michael Hollerer[4], Philipp Hurdax[4], Daniel Lüftner[4], Peter Puschnig[4], Georg Koller[4], Michael Ramsey[4], Moritz Sokolowski[3], Frank Stefan Tautz[1,2], and Serguei Soubatch[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, Germany — [3]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Germany — [4]Institut für Physik, Universität Graz, NAWI Graz, Austria

The electronic states and geometric vertical structures of perylene-tetracarboxylic dianhydride (PTCDA) molecule upon an oxygen-reconstructed $(\sqrt{2} \times 2\sqrt{2})$R45° Cu(100) surface are investigated using ARPES and the NIXSW technique, respectively. The orbital tomography measurement found that, in contrast to PTCDA on intrinsic Cu(100) where strong molecule-substrate interactions are present [1], the oxygen adsorbed on Cu(100) prevents change transfer from metal substrate into the PTCDA molecule. Further, the geometry of the PTCDA layer on the oxygen-recontructed surface is determined to be flat with a high adsorption height. The results corroborate that the oxygen simultaneously induces electronic and structural decoupling at the molecule-metal interface.

[1] D. Lüftner et al., Physical Review B 96, 125402 (2017)

O 109.4 Fri 11:15 MA 004

Thermally-activated Self-assembly and In Situ Oxidation of a Reduced Decaazapentacene — David Miklik[1], •Fatemeh Mousavi[2], Aisha Ahsan[2], Anna Middleton[3], Yoshitaka Matsushita[1], Jan Labuta[1], Paul Karr[5], Pavel Svec[1,6], Filip Bures[7], Gary Richards[1,8], Francis Souza[3], Thomas Jung[1,4], and Jonathan Hill[1] — [1]MANA-NIMS, Tsukuba, Japan — [2]University of Basel, Switzerland — [3]University of North Texas, USA — [4]Paul Scherrer Institute, Switzerland — [5]Wayne State College, USA — [6]Institute of Macromolecular Chemistry, Praha, Czech Rep. — [7]University of Pardubice, Czech Rep. — [8]Ochanomizu University, Otsuka, Japan

The higher pyrazinacenes are a newly synthesized class of molecules which may take an important role in organic semiconductors. This is due to their expected n-type behaviour which complements to the already important p-type pentacene derivatives with their closely related molecular structure. We report on the supra-molecular interactions and self-assembly of octaazatetracene and decaazapentacenes, two different lengths molecules in this class. On atomically clean Cu(111) the initially achiral compounds take a chiral conformation upon adsorption. Both compounds are imaged individually and form structurally related chains. Dehydrogenation occurs upon thermal activation as recognized by its stronger adsorption in the form of individual units. This on-surface reaction is compared to the dehydrogenation in solution. Experimental evidence is provided by Scanning Tunneling Microscopy and X-ray Photoelectron Spectroscopy.

O 109.5 Fri 11:30 MA 004

Aggregation by Metallophilic Interaction — •Michael Györök[1], Sebastian Wolfmayr[1], Petra Gründlinger[1,2], Uwe Monkowius[3], Peter Zeppenfeld[1], and Thorsten Wagner[1] — [1]Johannes Kepler University, Experimental Physics, Linz, Austria —

[2]Johannes Kepler University, Inorganic Chemistry, Linz, Austria — [3]Johannes Kepler University, School of Education, Linz, Austra

Metallophilicity describes attractive interactions between two or more metal atoms with closed shell configurations (i.e. d^8, d^{10}). Metal complexes containing gold in the formal oxidation state +I show very strong attractions, which are therefore also referred to as aurophilicity [1,2]. As a result, the aurohilic interactions determine often the arrangement of gold(I) complexes in the solid state. However, there are almost no examples in the literature, where this attractive interaction has been studied on surfaces. 2-naphthyl-isonitrile-gold(I)-chloride is and stable enough to sublime under ultrahigh vacuum conditions at moderate temperatures of 400 K. Ultrathin films of this molecule were prepared by physical vapor deposition on Au(111) surfaces. The deposition was monitored by differential reflectance spectroscopy (DRS) and photoelectron emission microscopy (PEEM). Finally, the structure of the organic film was analyzed by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) confirming an anti-dimer structure similar to the known bulk structure.

[1] P. Pyykkö, Chem. Rev. 97, 597 (1997).

[2] F. Schwerbaum *et al.*, Angew. Chemie 27, 1544 (1988).

O 110: New Methods: Theory

Time: Friday 10:30–10:45 Location: MA 005

O 110.1 Fri 10:30 MA 005

Error propagation in first principles kinetic Monte Carlo models — Sandra Döpking and •Sebastian Matera — Institut f. Mathematik, Freie Universität Berlin

The last years have seen an increasing interest in (chemical) kinetic models which have been parametrized using first principles electronic structure calculations. While these allow to access material properties without fitting the model to experimental data, commonly employed electronic structure theories rely on some approximations and thereby the estimated parameters carry an usually sizeable error. Using a first principles kinetic Monte Carlo model for the CO oxidation on the $RuO_2(110)$ surface as a example, we will address the propagation of these errors to the kinetic model's output. For this, we will employ a newly developed distribution based approach to global sensitivity analysis. This approach allows to estimate all sensitivity indices from a single set of sampling points of the parameter space and is also applicable to stochastic model outputs. Further, the resulting sensitivity indices might be interpreted as induced uncertainty by the respective uncertain parameter. For the model at hand, we find sizeable uncertainties but also that only a subset of all errors control this. Such information might be used to identify those parameters which are worth a determination with a more accurate electronic structure method or for identifying suitable descriptors for materials screening.

O 111: Oxides and Insulators: Adsorption II

Time: Friday 10:30–12:30 Location: MA 041

O 111.1 Fri 10:30 MA 041

New Insights into the Catalytic Activity of Solid Solutions: Carbon Dioxide Activation on NiMgO — •Aliaksei Mazheika, Marie-Mathilde Millet, Sabine Wrabetz, Elias Frei, Robert Schlögl, and Sergey V. Levchenko — Fritz-Haber-Institut der MPG, Berlin 14195, Germany

Ni_xMg_yO solid solutions are stable and active catalysts for dry reforming of CH_4 and CO_2 hydrogenation. Despite numerous experimental investigations, the structure of NiMgO surfaces at realistic conditions was unclear. We present a combined hybrid DFT/experimental study of CO_2 adsorption at NiMgO surfaces. The DFT calculations are performed with the HSE(α) functional, where the fraction of exact exchange α is set to 0.3 based on a comparison of the HSE(α) and CCSD(T) embedded-cluster calculations. The periodic calculations reveal that Ni_{Mg} defects prefer to occupy low-coordinated sites (corners and steps) at the MgO (100) surface [1]. Thus, Ni doping promotes formation of such sites during synthesis of the solid solution. Indeed, IR experiments showed that the number of undercoordinated O sites at NiMgO surfaces is significantly increased compared to pristine MgO samples. The stabilization of (110) and reconstructed octopolar (111) surfaces by Ni doping reconciles theoretical results with microcalorimetry measuremenbts of CO_2 adsorption energies. The presence of Ni at steps and corners considerably decreases CO_2 adsorption energies compared to pure MgO which prevents the carbonation and allows further chemical transformations of CO_2.

[1] A. Mazheika and S.V. Levchenko, JPCC **120**, 26934 (2016)

O 111.2 Fri 10:45 MA 041

Electronic and Surface Chemical Properties of the Interface Diethyl Carbonate/Zirconia — •Markus Frericks, Natalia Schulz, Thomas Späth, Wolfram Jaegermann, and René Hausbrand — Oberflächenforschung, FB 11, TU Darmstadt, Deutschland

Interface phenomena and related reaction layers play a crucial role in the performance and stability of lithium ion batteries (LIB). Besides the study of naturally formed solid electrolyte interface (SEI) layers, artificial protection layers are investigated on their potential to improve the stability of interfaces in LIBs. Among several candidates, zirconia (ZrO_2) was found to improve the cycle stability when used as thin film coating for cathode materials such as lithium cobalt oxide ($LiCoO_2$). While previous studies focused on the discussion of the high fracture toughness of ZrO_2 and thus mainly mechanical properties, we investigated the electronic and surface chemical properties of zirconia coated model electrodes by solvent adsorption.

The experiment was performed at the beam line UE56_PGM-1 at the photon source BESSY II in Berlin. Diethyl Carbonate (DEC), a commonly used solvent in the electrolyte of LIBs, was adsorbed in consecutive steps on a cooled sample of a thin ZrO_2 layer on a Ti substrate. The steps were monitored by X-ray photoelectron spectroscopy, yielding the electronic and chemical structure at the interface. Compared to the adsorption on pristine $LiCoO_2$, less reactions are observed. The results will also be discussed with respect to electron transfer through the layer system $LiCoO_2/ZrO_2$/DEC, evaluating the possibility for improved passivation by zirconia.

O 111.3 Fri 11:00 MA 041

Corrosion mechanism in lead-free materials for the electronic industry — •Gabriele Saleh and Stefano Sanvito — Trinity College Dublin, College Green, Dublin 2, Ireland

Silver and tin constitute the major components (>99%) of alloys adopted to assemble printed circuit boards, ever since many countries have severely restricted the use of lead due to its toxicity. However, those alloys tend to suffer from corrosion issues, which represent an economic burden for the electronic industry. Although Ag-Sn surfaces play the main role in the corrosion process, their structure, composition and reactivity have never been investigated at the atomic level. In this contribution, we show how we bridged this gap by means of extensive ab initio simulations [Saleh et al., PCCP, submitted]. We investigated more than 70 surfaces (including non-stoichiometric ones) for all the known Ag-Sn alloys, thereby establishing which surfaces are most stable and will form in a real sample. Moreover, we systematically studied O and S chemisorption, and contextualized the results in the framework of corrosion tendency. The observed trends are rationalized in terms of structural and electronic features. Calculations on suitable model systems were performed to confirm the proposed rationale. On top of that, we present our preliminary results on molecular dynamics simulations ('ReaxFF' approach) to address what we call 'silver paradox', that is the experimentally observed preferable formation of silver sulphide over silver oxide despite O and S having almost identical chemisorption energies on Ag and Ag2S and Ag2O formation energies being almost identical.

O 111.4 Fri 11:15 MA 041

Temperature dependent initial sticking probability of Mg atoms on H:Si and SiO2 surfaces — •Miriam Fritscher[1], Ulrich Hagemann[2], and Hermann Nienhaus[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg — [2]Interdisciplinary center for analytics on the nanoscale (ICAN), CENIDE, Duisburg

The temperature dependence of the initial sticking probability of magnesium atoms evaporated from a Knudsen-cell onto hydrogen passivated silicon (H:Si(111)) and silicon dioxide (SiO2)substrates is investigated. Mg is evaporated stepwise onto both surfaces simultaneously and X-ray photoelectron spectra are recorded after each step to determine the growth rate of the Mg film. This is done at variable substrate temperatures between 140 K and room temperature. It was found that the sticking probability of Mg atoms is approximately the same for both surfaces at low temperatures (T<210 K), whereas for room temperature it reaches zero for the SiO2 substrate. The temperature dependence of the sticking probability on Si surfaces is significantly smaller. Furthermore, the reduction of the sticking probability on SiO2 at room temperature is not dependent on the thickness of the SiO2 film. Experiments indicate that a single monolayer of SiO2 on Si results already in the dramatic decrease of the sticking probability. Once Mg atoms are sticking to the substrate they form islands and do not desorb again. A simple precusor mediated sticking-desorption model is applied to explain the findings.

O 111.5 Fri 11:30 MA 041

Interaction of an Ionic Liquid Adlayer with Spinel $Li_4Ti_5O_{12}$ and Influence of 1 Post- and Predeposited Lithium — •Jihyun Kim[1], 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

In this model study, we aimed toward a detailed understanding of the interaction of the battery-relevant ionic liquid 1-butyl-1-methylpyrrolidinium bis-(tri-fluoro-methyl-sulfonyl)-imide ([BMP][TFSI]) with well-defined spinel lithium titanate $Li_4Ti_5O_{12}(111)$, which is a promising anode material for a lithium-ion batteries, employing X-ray photoelectron spectroscopy (XPS) in ultrahigh vacuum (UHV). Furthermore, the influence of pre- and post-deposited Li on the IL adlayer was investigated. First of all, [BMP][TFSI] mainly adsorbs as intact ion pairs on $Li_4Ti_5O_{12}$ at 300 K, except a negligible amount of decomposition products (LiF, Li_xS, Li_xSO_y, SO_x and LiN_3), which increases moderately after post-deposition of 1 ML of Li, i.e. most of the Li most likely diffuses through the IL adlayer and subsequently into the bulk of $Li_4Ti_5O_{12}$. At 80 K, in contrast, a small amount of Li^+ remains in the near-surface regime, forming a Li-rich $Li_{4+x}Ti_5O_{12}$ (x ∼ 0.3) phase. Due to the remaining Li in the near surface, the subsequent deposition of the IL results in a significant decomposition of the adlayer, which demonstrates the reactive interaction of Li with the IL adlayer even at 80 K.

O 111.6 Fri 11:45 MA 041

Measuring Heats of Adsorption of Porphyrins on Oxide Single-Crystal Surfaces — •Ole Lytken, Quratulain Tariq, Daniel Wechsler, Matthias Franke, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Germany

Porphyrins are large organometallic complexes interesting for a variety of applications such as organic electronics and solar cells. For many of these applications the interface between the porhyrins and the substrate they are deposited on is particularly interesting. However, determining the heats of adsorption of porphyrins on surfaces is not straight forward: theoretical calculations have to include van der Waals interactions, and experimental measurements have to consider decomposition of the monolayer simultaneous with desorption. In this study we present temperature-programmed desorption (TPD) measurements of three porphyrins, CoTPP, ZnTPP and MgTPP, from an Mgo(100) surface. To reduce the influence of decomposition, which may affect the shape of the desorption peak, we use simple Redhead analysis. The accuracy of Redhead analysis depends critically on the chosen prefactor, and we use the prefactor derived from desorption of multilayers.

O 111.7 Fri 12:00 MA 041

Reversible and Efficient Photo-Switching of Azobenzene Derivatives on an Insulator Surface — •Simon Jaekel[1], Antje Richter[2], Robert Lindner[2], Christophe Nacci[1], Angelika Kühnle[2], Stefan Hecht[3], and Leonhard Grill[1] — [1]Department of Physical Chemistry, Karl-Franzens University of Graz, Austria — [2]Institute for Physical Chemistry, Johannes-Gutenberg University Mainz, Germany — [3]Department of Chemistry, Humboldt-University Berlin, Germany

Studying single molecular switches is of interest for a better understanding of fundamental physical and chemical processes, but also in view of their possible use in smart materials and molecular nanotechnology. Azobenzene is a prototypical molecular switch, which changes between trans and cis isomers at the central N=N bond upon an external stimulus. Adsorption on solid substrates allows to study their properties on the single-molecule scale. However, the mostly used metallic substrates can strongly influence the switching properties. Therefore, and also in view of potential electronic applications, the use of nonmetallic substrates is desired. Here, we report non-contact atomic force microscopy (nc-AFM) results on the first switching of individual azobenzene molecules on an insulating calcite surface. Surprisingly, cis isomers appear on the surface already directly after preparation, indicating kinetic trapping. It is demonstrated that unlike on metals the molecules retain their efficient photoisomerization properties known from solution. Furthermore, the photoisomerization is shown to be reversible and selective, depending on the excitation wavelength.

O 111.8 Fri 12:15 MA 041

C_{60} adsorption on a two-dimensional oxide quasicrystal — •Eva Maria Zollner[1], Stefan Förster[1], and Wolf Widdra[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The recent observation of a two-dimensional oxide quasicrystal (OQC) derived from ultrathin films of $BaTiO_3$ on Pt(111) demonstrates that quasicrystalline structures can emerge in the heteroepitaxial growth of conventional periodic materials [1]. Due to the complexity of QCs, studies on the relation between aperiodic order and physical properties are challenging. Therefore, QC surfaces have been tested as templates for the growth of two-dimensional single element QCs formed by molecular adsorbates [2]. Here we report the first adsorption studies on the $BaTiO_3$-derived OQC using C_{60} molecules. Different coverages of C_{60} have been deposited on the OQC at different temperatures and characterized by LEED and STM. At room temperature C_{60} molecules form hexagonal islands at the OQC surface with preferential adsorption at step edges, which indicates a weak interaction with the OQC substrate. At temperatures below 150 K the diffusion of individual C_{60} molecules is strongly suppressed and small C_{60} islands are formed upon adsorption. Besides local hexagonal C_{60} arrangements, we find local C_{60} structure with quadratic arrangement. The latter being combined into local triangle-square tilings.

[1] S. Förster et al., Nature 502, 215 (2013).

[2] J. A. Smerdon et al., Nano Lett. 14, 1184 (2014).

O 112: Electronic structure: Surface magnetism and spin phenomena II

Time: Friday 10:30–13:00 Location: MA 042

O 112.1 Fri 10:30 MA 042

Composite Kondo impurities created by assembly of entangled spin chains — •Sebastian Loth[1,2,3], Deung-Jang Choi[2,3,6], Roberto Robles[4], Shichao Yan[2,3], Jacob A. J. Burgess[2,3], Steffen Rolf-Pissarczyk[2,3], Jean-Pierre Gauyacq[5], Nicolas Lorente[6,7], and Markus Ternes[3] — [1]Universität Stuttgart, Institut für Funktionelle Materie und Quantentechnologien, Stuttgart — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart — [4]The Barcelona Institute of Science and Technology, ICN2, Barcelona, Spain — [5]Institut des Sciences Moleculaires d'Orsay, CNRS, Univ. Paris-Sud, Orsay Cedex, France — [6]Centro de Fisica de Materiales, CFM/MPC, San Sebastian, Spain — [7]Donostia International Physics Center, San Sebastian, Spain

We create spin chains in which a strongly correlated Kondo state emerges from antiferromagnetic coupling among the atoms of the chain [1]. We used a low-temperature scanning tunneling microscope to construct chains of Fe and Mn atoms on a copper nitride surface on Cu(100). Neither Fe nor Mn are Kondo-screened individually at the temperature of our experiment [2], but composite chains of Fe and Mn can become Kondo-screened. We find that significant inter-atomic entanglement of all magnetic atoms is a requirement for the emergence of the Kondo state. The resulting Kondo resonance is spatially distributed along the chain and can be modified by varying their composition, length and lattice constant. [1] D.J. Choi et al., Nano Lett. 17 6203 (2017). [2] C.F. Hirjibehedin et al., Science 317 1199 (2007).

O 112.2 Fri 10:45 MA 042

Mechanically-tunable Kondo resonance in a single molecule subjected to the magnetic field reveals pitfalls in determination of the Kondo scale — •Martin Švec[1], Martin Žonda[2], Oleksandr Stetsovych[1], Richard Korytár[2], Markus Ternes[3], Tomáš Novotný[2], and Pavel Jelínek[1] — [1]Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Praha, Czech Republic — [3]Max-Planck-Institut fur Festkorperforschung, Stuttgart, Germany

We study both experimentally and theoretically the mechanically-tunable Kondo resonance using the low-temperature scanning tunneling microscope (STM) to control the coupling of an organic molecule to its underlying metallic substrate. Pulling the molecule with a half-filled orbital and spin 1/2 from the metal surface changes the molecule's magnetic properties from the highly-correlated Kondo-singlet state to the weakly-coupled spin-flip regime, where an externally applied magnetic field can lift the state degeneracy. We employ simulations using the numerical renormalization group (NRG) theory for a reliable quantitative description of the measured low-bias differential conductance spectra and extraction of the characteristic Kondo energy scale spanning about 15 orders of magnitude. We show that the commonly used Fermi-liquid-based (Frota) and perturbative (Appelbaum) fitting procedures can be rather safely used in their corresponding limits of the high correlations and weak coupling, respectively, but they can dramatically fail even without warning signs in the crossover regime.

O 112.3 Fri 11:00 MA 042

Absorption-site specific Kondo resonance observed in single molecule magnet $TbPc_2$ on Ag(111) — •Jack Hellerstedt, Ales Cahlik, Martin Svec, Mario Moro, and Pavel Jelinek — Czech Academy of Sciences Institute of Physics

The single molecule magnet bis(phthalocyaninato)terbium(III) ($TbPc_2$) has attracted steady research attention as an exemplar system for realizing molecule based spin electronics. Lattices of these molecules interact through the π-electrons in their Pc ligands, which manifests itself experimentally as a Kondo resonance in spectroscopy measurements. Understanding these interactions is crucial for their subsequent use in quantum computing schema. We studied $TbPc_2$ molecules evaporated in ultrahigh vacuum onto a single crystal Ag(111) surface, measured at 5K using combined scanning tunneling and non-contact atomic force microscopies (STM/ nc-AFM). Submolecular resolution achieved with a CO- functionalized tip offers unprecedented structural information, specifically regarding the two sub-lattices forming tight-packed $TbPc_2$ islands. Kondo resonances are observed on molecules absorbed as a second layer on the larger $TbPc_2$ islands: the presence or absence of the Kondo signature is exactly correlated with the sub-lattice absorption site. Spectroscopies taken with a CO-terminated tip showed the Kondo resonance shifted to the center of the ligand. The latest efforts to understand the structural origin of this site-specific Kondo resonance will be reported.

O 112.4 Fri 11:15 MA 042

Probing magnetic interactions between Cr adatoms on the β-Bi_2Pd superconductor — •Deung-Jang Choi[1,2,3], Carlos García Fernández[3], Edwin Herrera[4], Carmen Rubio-Verdú[3], Miguel M. Ugeda[3], Isabel Guillamón[4], Hermann Suderow[4], Jose Ignacio Pascual[3], and Nicolás Lorente[2,3] — [1]Centro de Fisica de Materiales, CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastian, Spain — [2]Donostia International Physics Center (DIPC), Donostia-San Sebastian, Spain — [3]CIC nanoGUNE, Donostia-San Sebastián, Spain — [4]Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Spain

Recently, the introduction of new impurity states in the superconducting gap has received a lot of attention. Indeed, the search of a new superconducting state dubbed topological superconductivity is strongly based in the combination of doping classical (s-wave) superconductors with magnetic impurities that arrange in a chiral fashion. Magnetic adatoms can be considered as impurities that weaken the binding of superconducting Cooper pairs leading to impurity levels in the gap: so-called Yu-Shiba-Rusinov (YSR) states. By using scanning tunneling microscope (STM), we present the first results of controlled single-atom manipulation to assemble a chain of Cr atoms on a Bi_2Pd superconductor. The interatomic distance between two Cr atoms is thoroughly explored revealing Cr-Cr interactions mediated by the superconductor for the first time[1]. ([1] Choi, D.-J. et al. arXiv:1709.09224)

O 112.5 Fri 11:30 MA 042

Spin excitations in a 4f–3d heterodimer on MgO — Aparajita Singha[1], •Fabio Donati[2,1,3], Fabian Donat Natterer[1], Christian Wäckerlin[1,4], Srdjan Stavric[5], Zoran Popovic[5], Zeljko Sljivancanin[5], François Patthey[1], and Harald Brune[1] — [1]Institute of Physics, Ecole Polytechnique Federale de Lausanne, Switzerland — [2]Center for Quantum Nanoscience, Institute for Basic Science, Korea — [3]Department of Physics, Ewha Womans University, Korea — [4]Nanoscale Materials Science, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland — [5]Vinča Institute of Nuclear Sciences, Serbia

Many alloys of transition metals (TM) of the first row and rare earth (RE) elements posses large magnetic anisotropy. Atomic-scale structures made by these elements are intriguing model systems to explore unconventional magnetic phases where structural relaxations and interface effects can play a crucial role. Here we use scanning tunneling microscopy spin-excitation spectroscopy to unravel the magnetic level structure and exchange coupling in the smallest RE-TM cluster, namely HoCo dimers adsorbed on ultrathin layers of MgO on Ag(100). We observe two spin-excitations at ±8 and ±20 meV, the former being detectable with spin-polarized tips only. We model their magnetic field dependence with an effective spin Hamiltonian to identify the level splitting and the relative contribution of the two atoms to the spin excitation signal. Combining these results with density functional theory, we infer a ferromagnetic coupling between Ho and Co, which is opposite to what is known for late 4f–3d bulk compounds.

O 112.6 Fri 11:45 MA 042

Impurity bands and magnetic interactions in the quantum anomalous Hall insulators (V,Cr):$(Bi,Sb)_2Te_3$ — •Thiago R. F. Peixoto[1], Sonja Schatz[1], Can Raphael Crespo-Vidal[1], Hendrik Bentmann[1], Kai Fauth[1], Martin Winnerlein[1], Steffen Schreyeck[1], Charles Gould[1], Karl Brunner[1], Arthur Ernst[2,3], Laurens W. Molenkamp[1], and Friedrich Reinert[1] — [1]Exp. Phys. VII, II and III, Universität Würzburg — [2]Max Planck Institute of Microstructure Physics, Halle (Saale) — [3]Institute for Theoretical Physics, Johannes Kepler Universität Linz, Austria

Recently we have reported on the fingerprint of the 3*d* impurity states in the valence band of the quantum anomalous Hall system

V:$(BiSb)_2Te_3$ by means of resonant photoemission spectroscopy (resPES) [1]. These states lie at the Fermi level and carry a significant magnetic moment, so that they are expected to promote a ferromagnetic superexchange interaction between the magnetic dopants via *pd* hybridization. Here we report x-ray magnetic circular dichroism (XMCD) measurements at the $L_{2,3}$ edges of both V- and Cr-doped $(BiSb)_2Te_3$ thin films. We show the ferromagnetic character of V and Cr 3*d* impurity bands at temperatures below 50 K. We compare our XMCD data with our valence band resPES results, which are supported by *ab initio* calculations of the density of states (DOS), and discuss the implications of V and Cr 3*d*-DOS to the magnetism of magnetically doped topological insulators.

[1] T. R. F. Peixoto *et al.*, Physical Review B **94**, 195140 (2016).

O 112.7 Fri 12:00 MA 042

Interaction between spin waves and domain walls in ferromagnetic nanostripes — •Nerea Ontoso[1,2], Luis Lopez-Diaz[1], Luis Torres[1], and Rocio Yanes[1] — [1]University of Salamanca, Salamanca, Spain — [2]CIC nanoGUNE, San Sebastian, Spain

Spin waves are linear low-energy excitations that propagate in ferromagnetic materials. Domain walls, on the other hand, are very stable localized structures that separate regions with uniform magnetization. Both of them are key elements of various spintronic devices, such as racetrack memories or magnon transistors.

By using micromagnetic simulations, we study the interaction between domain walls and spin waves. We analyze two different cases: (i) a head-to-head domain wall in an in-plane magnetized soft ferromagnetic stripe and (ii) a Bloch wall in a nanostripe with high perpendicular anisotropy. We perform a systematic study as a function of the frequency, spin wave amplitude and distance between the spin wave source and the domain wall. We obtain a rather complicated frequency dependence that we try to interpret in terms of spin wave reflection/transmission at the domain wall. However, a general description of this process is complex and requires taking into account dipolar fields, excitation of internal domain wall modes and high order spin wave modes due to the finite stripe width.

O 112.8 Fri 12:15 MA 042

A first principle-based multiplet description of magnetic adatoms — •Fernando Delgado[1] and Jhon Wilfred González[2] — [1]Departamento de Física, Universidad de La Laguna, Instituto de estudios avanzados (IUdEA), Avda. Astrofísico Francisco Sánchez, S/N 38203 La Laguna (Tenerife), Spain — [2]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, Manuel de Lardizabal 5, E-20018 Donostia-San Sebastián, Spain

Magnetic atoms absorbed on surfaces has become a particularly attractive system to study the principles of quantum magnetism, in addition to their core interest for digital data storage. From a theoretical perspective, the simulation of these systems is quite challenging. Quite frequently, a density functional theory (DFT) calculation is used to extract the magnetic moments and magnetic anisotropy energy (MAE). Unfortunately, this description fails quite often even at qualitative level in describing the easy axis of the nanomagnet or the MAE. A much better description can be obtained by a dynamical mean field theory calculation, but at a considerably larger computational cost.

Here we have implemented an alternative description in the spirit of the multiplet calculations used in XMCD. A planewave-based spin-unpolarized DFT calculation is carried out to estimate, in combination with a maximally localized Wannier functions calculation, the crystal and ligand fields felt by the adatom electrons. This single electron picture is complemented by a many body exact configuration interaction method to extract the excitation spectra of the correlated system, together with the spin and orbital magnetic moments.

O 112.9 Fri 12:30 MA 042

Magnetism of thin Cr and Mn films on W(100) — •Matthias Vogt[1], Martin Schmitt[1], Ryan Cotsakis[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]The University of British Columbia, 2329 West Mall, Vancouver, BC, Canada V6T 1Z4

In this contribution we present spin-polarized scanning tunneling microscopy (SP-STM) data of thin Cr and Mn films on W(001). Due to strong spin-orbit coupling in the W substrate a significant Dzyaloshinskii-Morija interaction (DMI) can be expected, potentially leading to spin structures which are very different from those found in corresponding bulk materials. Quite contrary to this expectation, our results obtained on monolayer and double-layer Cr films on W(001) show an antiferromagnetic order between adjacent terraces, comparable to earlier observations on (001) surfaces of bulk Cr [1,2]. For the Mn double-layer on W(001) our SP-STM data show a checkerboard-like $(\sqrt{2} \times \sqrt{2})$ spin structure with an in-plane easy axis, largely reminiscent of the magnetic state previously found on the Fe monolayer on W(001), but very different from the spin spiral observed for the Mn monolayer on W(001) [3,4].

[1] M. Kleiber *et al.*, Phys. Rev. Lett. **85**, 4606 (2000).
[2] R. Ravlić *et al.*, Phys. Rev. B **67**, 174411 (2003).
[3] A. Kubetzka *et al.*, Phys. Rev. Lett. **194**, 087204 (2005).
[4] P. Ferriani *et al.*, Phys. Rev. Lett. **101**, 027201 (2008).

O 112.10 Fri 12:45 MA 042

Revealing the interplay between surface reconstruction and magnetic order in Fe bilayers on Ir(111) — •Nadine Hauptmann[1], Melanie Dupé[2], Tzu-Chao Hung[1], Alexander K. Lemmens[1], Jairo Sinova[2], Stefan Heinze[3], Daniel Wegner[1], Bertrand Dupé[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, Netherlands — [2]Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany — [3]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Chiral magnets, e.g. magnetic skyrmions have attracted heavy interest due to their potential application for nano-scale magnetic storage. Their stabilization depends on the interplay between mainly the magnetic exchange and Dzyaloshinskii-Moriya interaction. The latter one strongly depends on the geometric structure. A vast majority of atomic-scale studies have utilized spin-polarized scanning tunneling microscopy (SP-STM). However, with SP-STM it is difficult to distinguish between structural corrugation and electronic and magnetic properties. We use a recently developed combination of SP-STM and magnetic exchange force microscopy (SPEX) to study the spin spirals in the reconstruction line network in a bilayer Fe on Ir(111). We show that with SPEX and DFT calculations we can obtain a detailed understanding of both the structure and the electronic and magnetic properties. Our work is important to understand the origin of magnetic order in atomic-scale magnetic non-collinear systems.

O 113: 2D materials beyond graphene: TMDCs, silicene and relatives V

Time: Friday 10:30–13:00 Location: MA 043

O 113.1 Fri 10:30 MA 043

Growth and electronic structure of Sb bilayers on Bi2Se3: a route to achieve buckled antimonene — •Sanjoy K. Mahatha[1,2], Kris Holtgrewe[3], Roberto Flammini[4], Conor Hogan[4], Marco Papagno[5], Alessandro Barla[1], Paolo Moras[1], Polina M. Sheverdyaeva[1], Stefano Colonna[4], Fabio Ronci[4], Simone Sanna[3], Ziya S. Aliev[6], Evgueni V. Chulkov[7], and Carlo Carbone[1] — [1]CNR-ISM, I-34149 Trieste, Italy — [2]Aarhus University, 8000 Aarhus C, Denmark — [3]University of Giessen, Germany — [4]CNR-ISM, I-00133 Roma, Italy — [5]Universita della Calabria, 87036 Arcavacata di Rende (CS), Italy — [6]Azerbaijan National Academy of Science, AZ1143 Baku, Azerbaijan — [7]Donostia International Physics Center, Basque Country, Spain

Hetero-structures consisting of topological insulators and two-dimensional (2D) materials represent an interesting system, where interfacial phenomena play a crucial role, thus allowing for innovative applications. Here, we will give a detailed account of the electronic and atomic structure of Sb bilayers on the Bi2Se3 surface, which has been investigated using scanning tunneling microscopy (STM), angle-resolved photoemission spectroscopy (ARPES) and ab-initio calculations. Our STM results univocally prove the wetting structure of Sb on Bi2Se3 with buckled honeycomb structure. ARPES measurements and calculated band structures show that the hybridization of Sb states with the Bi2Se3 substrate plays an important role in determining the spin-pattern of the surface localized electronic states.

O 113.2 Fri 10:45 MA 043

k-space indirect interlayer excitons in MoS_2/WSe_2 van der Waals heterostructures — •J. Kunstmann[1], F. Mooshammer[2], P. Nagler[2], A. Chaves[3,4], F. Stein[1], N. Paradiso[2], G. Plechinger[2], C. Strunk[2], C. Schüller[2], G. Seifert[1], D. R. Reichman[4], and T. Korn[1] — [1]TU Dresden, DE — [2]Universität Regensburg, DE — [3]Universidade Federal do Ceara, BRA — [4]Columbia University, USA

In heterobilayers of transition metal dichalcogenides (TMDCs) a new type of exciton emerges, where electron and hole are spatially separated. These interlayer excitons allow exploration of many-body quantum phenomena and are ideally suited for valleytronic applications. Mostly, a basic model of fully spatially-separated electron and hole stemming from the K valleys of the monolayer Brillouin zones is applied to describe such excitons. Here, we combine photoluminescence spectroscopy and first principle calculations to expand the concept of interlayer excitons. We identify a partially charge-separated electron-hole pair in MoS_2/WSe_2 heterostructures residing at the Γ and K valleys. We control the emission energy of this new type of k-space indirect, yet strongly-bound exciton by variation of the relative twist angle. These findings represent a crucial step towards the understanding and control of excitonic effects in TMDC heterostructures and devices.

O 113.3 Fri 11:00 MA 043

Material Realistic Description of Coulomb Engineered Two-dimensional Materials — •Christina Steinke[1,2], Malte Rösner[3], Dmitry Ryndyk[2], and Tim 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, California 90089-0484, USA

Heterojunctions are building blocks of various applications in modern optoelectronics. Common heterojunctions rely on interfaces of different materials in order to gain the desired spatial band-gap modulations. We investigate a new type of lateral heterojunction imprinted externally into an otherwise homogeneous monolayer of a 2d material. In 2d semiconductors the Coulomb interaction can modify band gaps on an eV scale and can be drastically manipulated by external screening. This allows to tune the local band gaps within a monolayer by laterally structured dielectric surroundings and leads to characteristics of a heterojunction in the local density of states with a spatially sharp band gap modulation. By means of ab-initio calculations we study the nature and tunability of this band-gap modulation in 2d semiconductors in dependence of the chosen environment. Therefore we place a homogeneous monolayer on different laterally structured substrates. We identify optimal candidates for Coulomb engineered 2d systems and study their electronic transport properties depending on external electrical fields and charge doping.

O 113.4 Fri 11:15 MA 043

Strain-induced Formation of Grain Boundaries in the 2D Quantum Spin Hall State in WSe_2 — •Charlotte Herbig[1], Zahra Pedramrazi[1], Madeleine Philips[2], Dillon Wong[1], Yi Chen[1], Hsin-Zon Tsai[1], Shujie Tang[3], Hyejin Ryu[4], Artem Pulkin[5], Zahid Hussain[4], Sung-Kwan Mo[4], Zhi-Xun Shen[3], Oleg Yazyev[5], Eugene Mele[2], and Michael F. Crommie[1] — [1]University of California Berkeley — [2]University of Pennsylvania — [3]Stanford University — [4]Lawrence Berkeley National Lab — [5]École Polytechnique Fédérale de Lausanne

Monolayers of group VI transition metal dichalcogenides with chemical formula MX_2, where M stands for Mo or W and X is S, Se, or Te, come in different structural polymorphs such as 1H, 1T, and 1T'. The metastable 1T' phase of WSe_2 hosts exotic physical properties such as the existence of a 2D topologically non-trivial quantum spin Hall state. The low-symmetry 1T' phase is structurally degenerate and has three orientation variants. Using the atomically sharp tip of a scanning tunneling microscope, we induce strain on monolayer islands of 1T'-WSe_2 and thereby switch between these three orientations, creating and rearranging grain boundaries between two topologically non-trivial 1T' phases. The electronic structure of these grain boundaries is then explored via scanning tunneling spectroscopy and compared with calculations of confined electronic modes on the grain boundary.

O 113.5 Fri 11:30 MA 043

Probing the band structure of quasi-freestanding monolayer MoS_2 — •Clifford Murray[1], Wouter Jolie[1,2], Joshua Hall[1], Carsten Busse[1,2,3], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster — [3]Department Physik, Universität Siegen

We epitaxially grow high-quality molybdenum disulfide (MoS_2) monolayers on graphene on Ir(111), and probe its electronic structure with low temperature scanning tunnelling spectroscopy (STS).

A bandgap of 2.50 ± 0.05 eV is measured by STS, showing the freestanding nature of MoS_2 on this substrate. Furthermore, by combining constant height and constant current STS modes and measuring the state-resolved tunnelling decay constant [1], we are able to disentangle the contributions of states located at various high-symmetry points, such as the spin-split valence band at the K-point. The band structure is found to be in close agreement with theoretical calculations for freestanding MoS_2, further evidencing the weak coupling with its Gr/Ir(111) substrate. Additionally, the valence band is seen to undergo a stepwise bending towards twin boundary line defects in the MoS_2 layer - to the best of our knowledge a phenomenon not yet reported in this material.

[1] Zhang, C. et al, Nano Lett. 15, 6494 (2015)

O 113.6 Fri 11:45 MA 043

Evolution of defects in two-dimensional $MoTe_2$: from point to extended defects — •Mahdi Ghorbani-Asl[1], Tibor Lehnert[2], Janis Köster[2], Hannu-Pekka Komsa[3], Ute Kaiser[2], and Arkady Krasheninnikov[1,3] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Electron Microscopy Group of Materials Science, University of Ulm, Ulm 89081, Germany — [3]Department of Applied Physics, Aalto University, P.O. Box 11100, 00076 Aalto, Finland

Defects frequently govern the characteristics of solids, e.g., mechanical or optical properties. They also provide an efficient way to engineer materials properties, similar to doping in semiconductors. Using first-principles calculations combined with high-resolution transmission electron microscopy experiments, we study creation, agglomeration, and evolution of vacancies in monolayer $MoTe_2$ under electron irradiation. Various types of point and extended defects are studied and their atomic structures and formation energies are determined. The stability of flower-like defects and trefoil-like defects are compared with the line vacancies. Our results show that single Te vacancies have a tendency for agglomeration into vacancy lines. The stability of line defects is also found to be dependent on their orientation. We have also studied the effects of uniaxial and biaxial strain on the stability and dynamics of line defects. Our electronic structure calculations show that the defects can change the electronic properties of MoTe$_2$, suggesting new opportunities for defect engineering in these layered materials.

O 113.7 Fri 12:00 MA 043

Insights into ferecrystalline layered heterostructures using surface science techniques — •Fabian Göhler[1], Niels Rösch[1], Erik Hadland[2], Danielle Hamann[2], 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

The stacking of single sheets of 2D materials to design hybrids with new emergent properties is a rapidly emerging field in materials science. An interesting avenue to synthesize a large number of different layered heterostructures on a wafer scale is provided by the Modulated Elemental Reactants (MER) technique, which allows independent control over constituents and layering sequence. $[\mathrm{MX}_{1+\delta}]_m[\mathrm{TX}_2]_n$ ferecrystal heterostructures are nanocrystalline, turbostratically disordered, layered materials that are synthesized by MER from structurally modulated, amorphous precursors at relatively low temperatures.

The talk will give an overview over recent results obtained from surface science techniques, mainly X-ray photoelectron spectroscopy (XPS) and LEED, on a number of ferecrystal compounds. These techniques provide insight into electronic interactions and structural modulations within and in between distinct layers. Among the results shown are interlayer charge transfer in $[\mathrm{PbSe}_{1+\delta}]_1[\mathrm{NbSe}_2]_2$ and $[\mathrm{SnSe}_{1+\delta}]_m[\mathrm{TiSe}_2]_2$, antiphase boundaries in rocksalt-like BiSe bilayers separated by NbSe$_2$ or MoSe$_2$, and structural polytypism in single layers of MoSe$_2$ separated by BiSe.

O 113.8 Fri 12:15 MA 043

Lateral and Vertical Heterostructures of h-GaN/h-AlN: Electron Confinement, Band Lineup, and Quantum Structures — •Engin Durgun, Abdullatif Onen, Deniz Kecik, and Salim Ciraci — Bilkent University - UNAM, Bilkent Ankara Turkey

Lateral and vertical heterostructures constructed of 2D h-GaN and h-AlN display novel electronic and optical properties and diverse quantum structures to be utilized in 2D device applications. Lateral heterostructures formed by periodically repeating narrow h-GaN and h-AlN stripes, which are joined commensurately, behave as composite semiconducting materials. Direct-indirect characters of the band gaps and their values vary with the widths of these stripes. However, for relatively wider stripes, electronic states are confined in different stripes and make a semiconductor-semiconductor junction with normal band alignment. This way 1D multiple quantum well structures can be generated with electrons and holes confined to h-GaN stripes. Vertical heterostructures formed by thin stacks of h-GaN and h-AlN are composite semiconductors with a tunable fundamental band gap. However, depending on the stacking sequence and number of constituent sheets in the stacks, the vertical heterostructure can transform into a junction, which displays staggered band alignment with electrons and holes separated in different stacks. Despite the complexities due to confinement effects, the band diagram of the heterostructures and band lineup are conveniently revealed from the electronic structure projected to the atoms or layers. Prominent features in the optical spectra of the lateral composite structures are observed.

O 113.9 Fri 12:30 MA 043

Nanoscale energy flow in 2D metal / 2D semiconductor heterostructures studied with femtosecond electron diffraction — •Thomas Vasileiadis, Daniela Zahn, Yingpeng Qi, and Ralph Ernstorfer — Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin, Germany

Having techniques for studying energy flow mechanisms in systems with nanoscale heterogeneities is essential for the development of future nanodevices. This task can be carried out using femtosecond electron diffraction (FED), a technique in which the lattice response to electronic excitations is probed by ultrashort electron bunches [1]. In this talk we will present FED studies of a 2D metal / 2D semiconductor heterostructure. Our samples consist of exfoliated multilayer flakes of WSe$_2$ with epitaxially grown Au on their surface. WSe$_2$ in contact with nanostructured Au is a promising material for optoelectronics. As an example, a recent study reported 20,000-fold enhancement of photoluminescence [2]. For a deeper understanding of energy flow in this system we have studied the laser-induced vibrational excitation of the individual materials by means of the Debye-Waller effect. Our results show that decoration with Au has significant effect on the optical properties and lattice dynamics of WSe$_2$.

[1] L. Waldecker, R. Bertoni, R. Ernstorfer, J. Appl. Phys. 117, 044903 (2015).

[2] Z Wang, et al. Nature Communications 7, 11283 (2016).

O 113.10 Fri 12:45 MA 043

Structural prediction of two-dimensional materials under strain — •Pedro Borlido[1], Conrad Steigemann[2], Nektarios Lathiotakis[3], Claudia Rödl[1], Miguel Marques[2], and Silvana Botti[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, GR-11635 Athens, Greece

Using a constrained global structural prediction method we performed an extensive investigation of the low density phases of two-dimensional carbon and silicon. As expected, we find that graphene is stable for a large range of biaxial strains, while more complex configurations becoming energetically more favorable at areas per atom above 3.12 Å^2. Two dimensional silicon presents a more complex phase diagram, which includes both haeckelite-like structures and dumbbell configurations. In particular, we find as the groundstate of two-dimensional silicon a novel structure formed by a honeycomb lattice with a few strategically positioned dumbbell atoms. This material is 218 meV/atom more stable than silicene and is a quasi-direct semiconductor with a band gap of around 1.11 eV and a very dispersive electron band. These properties should make it easier to synthesize than pristine silicene and interesting for a wealth of opto-electronic applications.

O 114: Nanostructures at surfaces: 1D and 2D structures and networks IV

Time: Friday 10:30–11:30 Location: MA 141

O 114.1 Fri 10:30 MA 141

Terminal Alkyne Coupling on a Corrugated Noble Metal Surface: From Controlled Precursor Alignment to Selective Reactions — •Tao Lin[1], Liding Zhang[1], Jonas Björk[2], Zhi Chen[3], Mario Ruben[3,4], Johannes Barth[1], and Florian Klappenberger[1] — [1]Physik-Department E20, Technische Universität München James-Franck-Str., 85748 Garching (Germany) — [2]Department of Physics, Chemistry, and Biology (IFM), Linköping University 58183 Linköping (Sweden) — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology 76344 Eggenstein-Leopoldshafen (Germany) — [4]IPCMS-CNRS University de Strasbourg 23 Rue de Loess, 67034 Strasbourg (France)

Surface-templated covalent coupling of organic precursors currently emerges as a promising route to the atom-precise fabrication of low-dimensional carbon materials. Here, we investigate the adsorption and coupling reactions of 4,4”-diethynyl-1,1’:4’,1”-terphenyl on Au(110) under UHV conditions by using scanning tunneling microscopy combined with density functional theory and kinetic Monte Carlo calculations[1]. Annealing induces both 1,2,4 asymmetric cyclotrimerization and homo-coupling, resulting in various reaction products including a previously unreported, surface-templated H-shaped pentamer. Further Analysis of the temperature dependent relative product abundances unravels that 1,2,4-trimerization and homocoupling proceed via identical intermediate species with final products depending on the competition of coupling to a third monomer vs. dehydrogenation. [1] Lin et al., Chem. Eur. J. 2017, 23, 15588.

O 114.2 Fri 10:45 MA 141

Assembly of robust holmium-directed 2D metal-organic coordination complexes and networks on the Ag(100) surface and on epitaxial MgO/Ag(100) layers — •Martin Uphoff[1], Raphael Hellwig[1], Georg Michelitsch[2], Karsten Reuter[2], Harald Brune[3], Florian Klappenberger[1], and Johannes V. Barth[1] — [1]Physics Department, TUM, Munich, Germany — [2]Faculty of Chemistry, TUM, Munich, Germany — [3]Institute of Physics, EPFL, Lausanne, Switzerland

We report the fabrication of novel lanthanide-directed metal-organic coordination networks (MOCNs) and complexes under UHV conditions on a clean Ag(100) surface. Utilizing STM we investigate the assembly behavior of single holmium atoms as coordination centers and 1,4-benzenedicarboxylic acid (TPA) as molecular linkers. The step-wise fabrication of the structures, as well as an organic precursor phase is described in detail. We observe two different phases of holmium-based metal-organic architectures. MOCNs as well as Ho-directed metal organic complexes can be fabricated and structural models are developed and confirmed by DFT calculations. The contributions of metal-ligand interactions, hydrogen bondings between adsorbed molecules and the role of molecule substrate interaction is analyzed. Furthermore, the metal-organic layers could be realized on magnesium oxide on Ag(100) to screen them from electronic influences of the metal surface. MgO monolayers of unprecedented quality allow the fabrication of metal-organic structures, which are similar to those on the bare silver in terms of their binding motifs and stoichiometry.

O 114.3 Fri 11:00 MA 141

On-surface transmetalation of porphyrins — Diana Hötger[1], •Markus Etzkorn[1,2], Claudius Morchutt[1], Patrick Alexa[1], Doris Grumelli[3], Jan Dreiser[4], Heriberto Fabio Busnengo[5], Paula Abufager[5], Sebastian Stepanow[6], Rico Gutzler[1], and Klaus Kern[1,7] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]Institut für Angewandte Physik, Technische Universität Braunschweig, Germany — [3]Universidad Nacional de La Plata, Argentina — [4]Paul Scherrer Institute, Swiss Light Source, Villigen, Switzerland — [5]Insituto de Física, Rosario, Argentina — [6]Swiss Federal Institute of Technology Zurich, Switzerland — [7]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, Switzerland

We have investigated the transmetalation of metal porphyrin monolayer networks self-assembled on Au(111) using X-ray absorption, scanning tunneling microscopy and DFT studies. In the X-ray absorption the coordinated metal centers show the expected clear multiplet structure as a result of the ligand field. When depositing Co on the networks formed by Fe-porphyrins at room temperature, we find strong evidence of an efficient metal cation exchange in the spectra. The Co absorption spectra now show a clear multiplet structure similar to the one of Co-porphyrins while the Fe spectra become much more metallic in character. The process is unidirectional as we find no signs of transmetalation for Fe deposited on Co-porphyrins. We have also observed similar signatures of transmetalation for Cu-porphyrins when depositing Co. The latter finding illustrates the differences to transmetalation in solution.

O 114.4 Fri 11:15 MA 141

Investigation of stepwise crosslinked 4-terphenylthiol self-assembled monolayers — •Patrick Stohmann, Sascha Koch, Yang Yang, Christopher David Kaiser, and Armin Gölzhäuser — Department of Physics, University of Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

When aromatic self-assembled monolayers (SAMs) are electron-irradiated, intermolecular crosslinking leads to the formation of Carbon Nano Membranes (CNM) with molecular thickness [1]. The present investigation focuses on the structural transformation from a pristine 4-terphenylthiol (TPT) SAM on Au(111), comparable to previous experiments [2], to a fully crosslinked molecular film, induced by a stepwise increase of the 50 eV electron irradiation dose. The amorphism of the respective partially crosslinked films is investigated by means of scanning tunneling microscopy (STM) at UHV conditions. Electron-induced chemical modifications of the molecular layer and the layer-gold interface as well as the change in the molecular order are investigated by X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED), respectively.

O 115: Molecular films: Photovoltaics, electronics and morphology (joint session O/CPP)

Time: Friday 10:30–11:30 Location: MA 144

O 115.1 Fri 10:30 MA 144

Excitonic states in films of 1,3-diphenylisobenzofuran — •Janek Rieger, Daniel Niesner, and Thomas Fauster — Lehrstuhl für Festkörperphysik, University of Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Films of 1,3-diphenylisobenzofuran (DPIBF) show singlet fission (SF), a mechanism for multi-exciton generation that might be used to enhance the efficiency of organic photovoltaics [1]. The yield of singlet fission depends strongly on the structural polymorph of the film [2]. We use ultraviolet photoelectron spectroscopy, monochromatic two-photon photoelectron spectroscopy, photoluminescence (PL) spectroscopy and time-resolved PL to investigate the occupied molecular orbitals and excitonic behavior in different polymorphs of DPIBF on Cu(111). Preparations under ultra-high vacuum conditions provided well-defined samples, on which in-situ measurements were carried out. In disordered films an excimer trapping state with a lifetime of 50 ns was found with an energy ~ 0.5 eV below the first excited singlet state S_1. For ordered films additional three vibrational progressions were found, which can be attributed to the S_1 excitons of two different polymorphs with energies of 2.62 eV and 2.66 eV and an emissive triplet pair species with an energy of 2.72 eV. The latter decays with two time constants in the subnanosecond regime. A relative PL yield < 0.12 was determined for the ordered films, which points towards a highly SF active film.

[1] M. C. Hanna, and A. J. Nozik, J. Appl. Phys. **100**, 074510 (2006).
[2] J. L. Ryerson et al., J. Phys. Chem. C **118**, 12121-12132 (2014).

O 115.2 Fri 10:45 MA 144

Polarized-Light Induced Contact Potential Differences in Small-Molecule Organic Aggregates and Thin Films — •Frank Balzer[1], Matthias Schulz[2], Oliya S. Abdullaeva[3], Arne Lützen[2], and Manuela Schiek[3] — [1]University of Southern Denmark, MCI, Sønderborg, Denmark — [2]University of Bonn, Germany — [3]University of Oldenburg, Germany

Crystalline organic thin films often exhibit linear dichroism and birefringence. Illumination with polarized light might therefore lead to polarization dependent changes of the electric surface potential. Here, we present results for birefringent and dichroic nanofibers from functionalized *para*-quaterphenylene molecules [1], and for thin films and thin film blends from an dihydroxy anilino squaraine (SQIB) [2]. Considerable differences in the light-induced changes of the surface potential are observed, probed by Kelvin probe force microscopy (KPFM). These changes are associated with the local molecule orientation within the samples.

[1] J. Chem. Phys. 146 (2017) 134704. [2] Cryst. Growth Des. (2017), doi: 10.1021/acs.cgd.7b01131.

O 115.3 Fri 11:00 MA 144

Work function variation due to electron induced conversion of self-assembled monolayers into carbon nano-membranes — Paul Penner[1], •Sascha Koch[1], Marcin Kiesiel[2], Thilo Glatzel[2], Emanuel Marchewski[1], Xianghui Zhang[1], Ernst Meyer[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, University of Bielefeld, 33615 Bielefeld, Germany — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland

For the realization and improvement of molecular electronic devices as for instance nano capacitors, the determination and specific tuning of electrical properties of the build-in materials plays an important role [1]. Our main research is focused on Carbon nano-membranes (CNMs), made by e.g. electron irradiation induced cross-linking of self-assembled monolayers (SAMs) of aromatic, organic molecules. Using different precursor molecules for the SAM preparation allows us to tune various properties of the resulting CNM [2]. Here, we present a material study about the change in the work function of pristine SAMs and CNMs on a Au(111) substrate by means of Kelvin Probe Force Microscopy (KPFM) for different precursor molecules. For different samples, the morphology as well as the work function of partially cross-linked and pristine SAM areas were compared, showing only differences in the contact potential (CPD). This effect can be attributed to the dipole moment modification of the molecular layer as well as the molecule-substrate interface but also to influences of different headgroup functionalizations. [1] X. Zhang et al., J.Appl.Phys. 2017, 122, 055103. [2] A. Turchanin et al., Adv. Mater. 2016, 28, 6075-6103.

O 115.4 Fri 11:15 MA 144

Local near-field spectroscopy of squaraine J-aggregates — •Jinxin Zhan, Jens Brauer, Manuela Schiek, Petra Gross, and Christoph Lienau — Carl von Ossietzky Universität, Oldenburg, Germany

Investigating the relationship between structure and function of organic molecular systems is of great interest for understanding their optical and electronic properties, inter- and intra-molecular coupling, and further applications such as solar cells, transistors, and photovoltaic devices. Optical microscopy on a nanometer length scale is one promising approach to obtain such insights. Here we employ scattering-type near-field scanning optical microscopy (NSOM) to probe the local spectrum of squaraine J-aggregates (R-ProSQ-C16). We model two resonances in the far-field spectrum of the molecules as transitions from the ground state to two excited states which originate from the energy level splitting caused by the coupling between two adjacent monomers. The splitting strength and hence the transition energy is determined by the tilt angle between the two coupled monomer dipoles. Near-field spectral measurements resolve local scattering spectra in 10-nm-radius domains. They reveal that the resonance energies measured in the individual domains vary from each other. These near-field spectral measurements, in combination with our theoretical modelling, reveal local variations in the tilt angle between the two monomer dipoles.

O 116: Focus Session: Structural Dynamics in Nanoscale Materials, Probed by Ultrafast Electron Pulses III

Time: Friday 10:30–12:45 Location: HE 101

Invited Talk O 116.1 Fri 10:30 HE 101

Imaging Coherent, Nanoscale Acoustic-Phonon Dynamics with Ultrafast Electron Microscopy — •David Flannigan, Daniel Cremons, Daniel Du, Dayne Plemmons, and Spencer Reisbick — University of Minnesota, Dept. of Chemical Engineering and Materials Science, Minneapolis, MN, USA

Here, I will describe our work on the development and the application of ultrafast electron microscopy [1]. I will begin with a brief overview of the UEM technology specific to our lab, focusing on imaging and operating at low instrument repetition rates. Following this, I will describe our progress in resolving the influence of nanoscale structural discontinuities on coherent, elastic strain-wave dynamics in a variety of materials [2-4]. For example, in transition-metal dichalcogenides, we find that wave trains emerge at extended discontinuities and that preferred propagation directions are independent of crystallographic orientation. In Ge, we find that individual phonon wave fronts propagate at hypersonic velocities and display a picosecond phase-velocity dispersion to the speed of sound. Overall, the observed dynamics indicate a single Lamb-type mode is excited several tens of picoseconds after femtosecond photoexcitation, suggestive of a link to charge-carrier dynamics via Auger recombination and the launch of electron-hole plasma waves.

[1] D. A. Plemmons and D. J. Flannigan, Chem. Phys. Lett. 683, 186 (2017). [2] D. R. Cremons, D. A. Plemmons, and D. J. Flannigan, Nat. Commun. 7, 11230 (2016). [3] D. R. Cremons, D. A. Plemmons, and D. J. Flannigan, Struct. Dyn. 4, 044019 (2017). [4] D. R. Cremons, D. X. Du, and D. J. Flannigan, Phys. Rev. Materials 1, 073801 (2017).

O 116.2 Fri 11:00 HE 101

Ultrafast TEM: probing nanoscale dynamics with coherent electron pulses — •Armin Feist[1], Nara Rubiano da Silva[1], Thomas Danz[1], Marcel Möller[1], Nora Bach[1], Katharina E. Priebe[1], Murat Sivis[1], Sascha Schäfer[1,2], and Claus Ropers[1] — [1]IV. Physical Institute, Universität Göttingen, Göttingen, Germany — [2]Institut für Physik, Universität Oldenburg, Oldenburg, Germany

Over the past decades, ultrafast techniques have shaped a rich picture of materials dynamics in spatially homogenous systems. Extending these concepts, ultrafast transmission electron microscopy (UTEM) combines the versatile imaging, diffraction and spectroscopy capabilities of state-of-the-art TEM with femtosecond temporal resolution achieved by a laser pump/electron probe scheme [1,2].

Here, we demonstrate local diffractive probing and phase-contrast imaging with nm-/fs- spatio-temporal resolution. The Göttingen UTEM instrument features photoemission from a nanoscale photocathode, delivering high coherence electron pulses of 0.6 eV energy width, down to sub-1 nm focal spot size, 200 fs pulse duration [2] and attosecond capability [3]. In particular, we employ ultrafast convergent beam electron diffraction (U-CBED) for the quantitative retrieval of the time- and space-dependent local deformation gradient tensor. Hereby, we map the optically induced acoustic lattice distortions, localized at the edge of a single-crystalline graphite thin film [4].

[1] A. H. Zewail, *Science*, **328**, 187 (2010). [2] A. Feist *et al.*, *Ultramicroscopy*, **176**, 63 (2017). [3] K. E. Priebe, *Nat. Photonics* **11**, 793 (2017). [4] A. Feist *et al.*, arXiv: 1709.02805.

O 116.3 Fri 11:15 HE 101

Generation of attosecond electron pulses via ponderomotive interaction with tailored light fields — •Martin Kozák[1,2], Timo Eckstein[1], Norbert Schönenberger[1], and Peter Hommelhoff[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstrasse 1, 91058 Erlangen, Germany, EU — [2]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic, EU

In this contribution we experimentally demonstrate the generation of attosecond electron pulse trains via a novel technique based on the inelastic ponderomotive scattering of electrons at an optical travelling wave created by two laser pulses at different frequencies. A large modulation of the kinetic energy of 29 keV electrons with a peak acceleration gradient of G=2.2 GV/m (energy gain/travelled distance) was observed using this technique [1]. After the interaction, a time-correlated energy modulation of the electrons leads to a ballistic compression due to the dispersive propagation of the electrons in vacuum. Detection of the sub-cycle temporal structure in the post-interaction electron distribution was performed via energy streaking using a second phase-controlled travelling wave interaction. Measured spectrograms and their comparison with numerical calculations allow monitoring the evolution of the electrons' longitudinal phase space distribution. In the temporal focal plane, attosecond electron pulse trains are formed with an individual pulse duration of 300 as. [1] Kozák, M., Eckstein, T., Schönenberger, N. & Hommelhoff, P., Nat. Phys. (2017), DOI: 10.1038/NPHYS4282.

O 116.4 Fri 11:30 HE 101

meV Resolution in Laser-Assisted Energy-Filtered Transmission Electron Microscopy — •Enrico Pomarico[1], Ivan Madan[1], Gabriele Berruto[1], Giovanni Maria Vanacore[1], Kangepeng Wang[2], Ido Kaminer[2], F. Javier García de Abajo[3,4], and Fabrizio Carbone[1] — [1]Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne CH-1015, Switzerland — [2]Andrew and Erna Viterbi Department of Electrical Engineering, Technion Israel Institute of Technology, 32000 Haifa, Israel — [3]ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain — [4]ICREA-Institució Catalana de Recerca i Estudis Avançats, Passeig Lluís Companys, 23, 08010 Barcelona, Spain

Dynamical characterization and manipulation of low energy excitations of quantum solids requires combining simultaneously nm-spatial, fs-temporal, and meV-spectral resolution.

We demonstrate a new method of spectrally-resolved photon induced near-field electron microscopy that allows us to obtain nm-fs resolved maps of nanoparticle plasmons with an energy resolution determined by the laser linewidth (20 meV in this work), and no longer limited by electron beam and spectrometer energy spreading (arXiv:1710.01183).

This technique can be extended to any optically-accessible low-energy mode, thus pushing TEM to a previously unattainable spectral domain with an unprecedented combination of space, energy, and temporal resolution.

O 116.5 Fri 11:45 HE 101

Time resolved X-Ray Photoelectron Diffraction of Quasi Freestanding Monolayer Graphene — •K Volckaert[1], D Kutnyakhov[2], M Bianchi[1], J Miwa[1], C Sanders[1], S Ulstrup[1], F Pressacco[2], G Brenner[2], K Medjanik[3], D Vasilyev[3], S Agustsson[3], Y-J Chen[8], F Speck[5], K Bühlmann[6], R Gort[6], F Diekmann[7], K Rossnagel[7], Y Acremann[6], T Seyller[5], C Tusche[4], H-J Elmers[3], G Schönhense[3], W Wurth[2], P Hofmann[1], and D Curcio[1] — [1]Aarhus University — [2]DESY Photon Science — [3]Johannes Gutenberg Universitat Mainz — [4]Forschungszentrum Jülich (FZJ) — [5]Technische Universitat Chemnitz — [6]ETH Zurich — [7]Christian-Albrechts-Universitat zu Kiel — [8]Universität Duisburg-Essen

We report the expansion for the first time of x-ray photoelectron diffraction (XPD) to the ultra-fast time domain by implementing it as a pump probe photoemission technique.

Conventional XPD has proven to be a powerful and efficient tool to probe structural order in matter. The expansion to the time domain allows the exploration of the structural dynamics in surfaces giving a completely new tool for the direct observation of surface structural dynamics.

The novel technique has been implemented at the FLASH free electron laser facility at DESY (Hamburg) by employing a time-of-flight momentum microscope, and it has been applied for the first time to give structural information on the dynamics of a quasi-freestanding monolayer graphene sample following excitation by a 800nm laser pulse.

O 116.6 Fri 12:00 HE 101

Femtosecond Electron Dynamics at the Single Atom Level — •Mohamad Abdo[1,2,3], Steffen Rolf-Pissarczyk[2,3], Björn Schlie[1,2,3], Luigi Malavolti[1,2,3], Jacob Burgess[3,4] und Sebastian Loth[1,2,3] — [1]Universität Stuttgart, Institut für Funktionelle Materie und Quantentechnologien, Stuttgart, Germany — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [4]Department of Physics and Astronomy, University of Manitoba, Winnipeg, Canada

Layered transition metal dichalcogenides (TMD) have complex electronic structure. Some of them as NbSe2 and TaS2, feature charge density wave (CDW) phases in which the electrons order with a periodicity that is incommensurate with the atomic lattice. Studies using optical pump probe techniques showed a picosecond response of the CDW [1] as well as a strong impact of pinning to atomic-sized defects [2]. Here we apply THz-coupled scanning tunneling microscopy [3] to measure the ultrafast dynamics of a CDW locally at individual atomic defects. Pairs of THz pulses excite the CDW and probe the response in the sample's density of states with a time resolution better than 200 fs. We find that the CDW responds to an excitation on a timescale well below 1ps and exhibits rich dynamics with a string spatial variation on the scale of one unit cell of the CDW. [1] X. Xi, et al. Nature Nanotechnology 10, 765-769 (2015) [2] P. Soumyanarayanan, PNAS 110, 1623-1627 (2013). [3] T. Cocker, et al., Nature Photonics 7, 620-625 (2013).

O 116.7 Fri 12:15 HE 101

Attomicroscopy: from femtosecond to attosecond electron pulse — •Mohammed Hassan — Physics Department, University of Arizona, Tucson, AZ, USA.

Ultrafast Electron Microscopy (UEM) has been demonstrated to be an effective table-top technique for imaging the atomic motion in real time and space. However, imaging the faster motion of electron dynamics has remained beyond the reach due to the lack of temporal resolution. Here, we demonstrate more than an order of magnitude (16 times) enhancement in the typical temporal resolution of UEM by generating isolated 30 fs electron pulses, accelerated at 200 KeV, via the optical-gating approach, with sufficient intensity for efficiently probing the electronic dynamics of matter in real time. Moreover, we explore the feasibility of attosecond optical gating to generate subfemtosecond electron pulses utilizing the optical attosecond pulse. which allow attaining the desired temporal resolution in electron microscopy for establishing the Attomicroscopy and image the electron motion in the act.

O 116.8 Fri 12:30 HE 101

Ultrafast electron diffraction in Troitsk: present state and perspectives — •Sergei Aseyev[1], Boris Mironov[1], Victor Kompanets[1], Anatoly Ischenko[2], Oleg Misochko[3], Sergei Chekalin[1], and Evgeny Ryabov[1] — [1]Institute of Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow, 108840 Russia — [2]Moscow Technological University, pr. Vernadskogo 86, Moscow, 119571 Russia — [3]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow region, 142432 Russia

The generation of coherent optical phonons in Sb film has been directly observed using table-top ultrafast electron diffractometer. The sample has been excited by a femtosecond laser pulse (λ = 800 nm) and probed with femtosecond photoelectron beam. Oscillations of the intensity corresponding to vibration frequencies of optical phonons excited by the laser have been observed in the obtained diffraction patterns: totally symmetric (A1g) and twofold degenerate (E2g) phonon modes of antimony and their combinations. Ultrafast electron diffraction method paves the way to study nonlinear phononics in perovskites and nonlinear photonics in molecular clusters.

O 117: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Friday 10:30–12:45 Location: HL 001

O 117.1 Fri 10:30 HL 001

Ab initio photoluminescence in 2D materials — •Pedro Melo[1,4], Andrea Marini[2,4], Matthieu Verstraete[1,4], and Zeila Zanolli[3,4] — [1]NanoMat / CESAM, ULiege Belgium — [2]ISM CNR, Italy — [3]RWTH Aachen Germany — [4]ETSF

The theoretical study of photoluminescence (PL) has been hindered in the past due to lack of predictive ab initio numerical techniques [1,2,4]. We present a complete theoretical framework for the computation of PL where electrons, nuclei, and photons are quantised. The intrinsic non-equilibrium nature of the process is fully taken into account [3]. Starting from the Keldysh contour, we arrive at a set of equations for the Green's functions of electrons, phonons, and photons where the different kinds of interactions are treated on the same footing. These equations are then simplified by using the generalised Baym-Kadanoff ansatz and the completed collision approximation [3]. This reduces the problem to a set of decoupled equations for the density matrix that describe all kinds of static and dynamical correlations. We show how the micro-macro connection relates the observable spectrum with the time-dependent microscopic dynamics, via the Bethe-Salpeter equation. Finally, we present the results of our numerical studies on 2D materials, such as WS2, where we relate the evolution of the carrier populations in the Brillouin zone with the changes in the PL spectrum of the material, for a range of experimental setups. [1] M. F. Pereira and K. Henneberger, PRB 58, 2064 (1998). [2] K. Hannewald, et al, PRB 67, 233202 (2003). [3] P. M. M. C. de Melo and A. Marini, PRB 93, 155102 (2016). [4] S. W. Koch, et al, Nat Mat 5, 523 (2006).

O 117.2 Fri 10:45 HL 001

Strain on molybdenum disulfide sheets with defects from first principles — •Mohammad Bahmani[1], Mahdi Faghihnasiri[2], and Thomas Frauenheim[1] — [1]BCCMS, Physics Department, Bremen

University, Bremen, Germany — [2]Physics Department, Shahrood University of Technology, Shahrood, Iran

Single layer of transition metal dichalcogenides(TMDCs) are under intense investigations since the discovery of unique characteristics of 2D and Vann der Waals layered materials. They are predicted to be the most promising structure for various future nanoscale devices. They have also novel applications in spintronic and optoelectronic. As a result of thermal equilibrium and the kinetics of processing, all real materials contain structural defects which show significant effects on their electrical, optical, vibrational, magnetic, and chemical properties. Besides, mechanical strain has very much influence on the electronic properties of 2D materials, particularly TMDCs. For example, 0.5% biaxial strain force direct band gap in molybdenum disulfide(MoS2) to become indirect since it breaks the crystalline symmetry. Therefore, I study different types of point defects such as single and double sulfur(S), single molybdenum(Mo) vacancies, and removing a Mo with its three upper S neighbors. I also substitute a Mo vacancy with one and two S atoms. Furthermore, as the second aim of this study, I showed the modification of defect states under uniaxial and biaxial compression and tensile strain. For the case of one S vacancy, this moves shallow states into the valance band and importantly breaks the degeneracy of degenerate states.

O 117.3 Fri 11:00 HL 001

Competion of magnetic interactions and in-field behavior of cycloidal Uranium compound UPtGe. — •Leonid Sandratskii — Max Planck Institute of Microstructure Physics, Halle, Germany

Stimulated by recent high-field experiment [1] performed on unique actinide system with cycloidal magnetic structure, UPtGe, I performed a series of calculations aiming to understand the nature of the sequence of magnetic phase transitions caused by the applied magnetic field. The physics of the system is determined by the fine balance of the exchange interaction, magnetic anisotropy, and Dzyaloshinskii-Moriya interaction. This balance of interactions governs, in particular, the in-field behavior of the system. The physical consequences of the variation of the localization of the U 5f electrons is investigated.

[1] A. Miyake, A. Nakamura, Y. Shimura, Y. Honma, D. Li, F. Honda, M. Tokunaga, D. Aoki, doi.org/10.11316/jpsgaiyo.71.1.0_2062.

O 117.4 Fri 11:15 HL 001

Electron correlation effects in the electronic structure of 4f-atoms adsorbed on metal and Graphene substrates — •Alexander B. Shick[1], Dmitry S. Shapiro[2], and Alexander I. Lichtenstein[3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]nstitute of Radio Engineering and Electronics, Russian Academy of Sciences, Moscow — [3]Institute of Theoretical Physics, University of Hamburg, Germany

Surface supported single magnetic atoms, the so-called "single-atom magnets", open new opportunities in a quest for the ultimate size limit of magnetic information storage. Initially, the research mainly focused on 3d-atoms on surfaces. Recently, the attention was turned to the 4f-atoms, culminating in the experimental discovery of magnetically stable Ho atom on MgO(001) substrate [1], and Dy atom on graphene/Ir(111)[2]. We address the electronic and magnetic character of 4f-atoms on metal and Graphene substrate making use of a combination of the DFT with the exact diagonalization of Anderson impurity model (DFT+ED) [3]. The spin and orbital magnetic moments of Dy@Ir(111) and Dy/Graphene/Ir(111) are evaluated and compared with experimental XMCD data. The magnetic anisotropy energy is estimated, and the magnetic stability is discussed. The role of 5d-4f interorbital exchange polarization in modification of the 4f-shell energy spectrum is emphasized. [1] F. Donati et al., Science 352, 318 (2016). [2] R. Baltic et al., Nano Lett. 16, 7610 (2016). [3] A. B. Shick, D. S. Shapiro, J. Kolorenc, A. I. Lichtenstein, Sci. Rep. 7, 2751 (2017).

O 117.5 Fri 11:30 HL 001

Interlayer trions in the MoS_2/WS_2 van der Waals heterostructure — •Thorsten Deilmann and Kristian Sommer Thygesen — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Electronic excitations in van der Waals heterostructures can have interlayer or intralayer character depending on the spatial localisation of the involved charges (electrons and holes). In the case of neutral electron-hole pairs (excitons), both types of excitations have been explored theoretically and experimentally. In contrast, studies of charged trions have so far been limited to the intralayer type.

Here we investigate the complete set of interlayer excitations in a MoS_2/WS_2 heterostructure using a novel ab-initio method, which allows for a consistent treatment of both excitons and trions at the same theoretical footing. Our calculations predict the existence of bound interlayer trions below the neutral interlayer excitons. We obtain binding energies of 18/28 meV for the positive/negative interlayer trions with both electrons/holes located on the same layer. In contrast, a negligible binding energy is found for trions which have the two equally charged particles on different layers.

O 117.6 Fri 11:45 HL 001

The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining — •Miguel Marques[1] and Antonio Sanna[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck Institut für Microstrukture Physics, Weinberg 2, 06120 Halle, Germany

Starting from the experimental data contained in the inorganic crystal structure database, we use a statistical analysis to determine the likelihood that a chemical element A can be replaced by another B in a given structure. This information can be used to construct a matrix where each entry (A,B) is a measure of this likelihood. By ordering the rows and columns of this matrix in order to reduce its bandwidth, we construct a one-dimension ordering of the chemical elements, analogous to the famous Pettifor scale. The new scale shows large similarities with the one of Pettifor, but also striking differences, especially in what comes to the ordering of the non-metals.

O 117.7 Fri 12:00 HL 001

Novel two-dimensional topological insulators from first principles materials screening — •Thomas Olsen and Kristian Thygesen — Technical University of Denmark

We have applied first principles calculations to find new stable two-dimensional materials with non-trivial band topology. The novel materials include more than 10 quantum spin Hall insulators, quantum anomalous Hall insulators and topological crystalline insulators protected by mirror symmetry. We also discuss the dual topological nature of the band structure in the presence of both time-reversal and mirror symmetry and show that odd mirror Chern numbers always imply a quantum spin Hall effect.

O 117.8 Fri 12:15 HL 001

Nanoparticles Classification with Self-Organisation Map (SOM) on 3D Electrostatic Potential Surface (EPS) — •Baichuan Sun and Amanda Barnard — Molecular & Materials Modelling, Data61 CSIRO, Door 34 Goods Shed, Village St, Docklands, VIC 3008, Australia

State-of-the-art deep learning (DL) algorithms are having tremendous impact across all scientific fields, and Material Science (MS) is no exception. A combination of computational chemistry simulations and DL techniques requires a hybrid computation/data research workflow, which represents a revolutionary approach to MS studies. There is a gap between the ab initio characterisation of nanomaterials with electronic structure simulations and its analytics with DL frameworks which stems from difficulties in representing quantum mechanical properties in such a way that is suitable for artificial neural networks. To overcome this issue we are evaluating the efficiency of visualising the 3-D Electrostatic Potential Surface (EPS) with Self-organising Maps (SOM), and integrating them directly into reliable DL frameworks. A Self-organisation Map classifies high-dimensional data into low-dimensional (normally 2D) space without supervision, while retaining the intrinsic topological relationship of the data set. As we will show, it is possible to represent a 3D molecular EPS with a single 2D snapshot, or "fingerprint" of the particle, provided they are orientationally invariant. In this study we demonstrate how Ag nanoparticles 3-D EPS self-organising texture maps can be used to classify nanoparticles based on the energy of the Fermi level.

O 117.9 Fri 12:30 HL 001

Regulation of structure and high thermoelectric performance of 1D SnTe via encapsulation within single-walled carbon nanotube — Andrij Vasylenko[1], •Jamie Wynn[2], Sam Marks[1], Paulo V. C. Medeiros[3], Quentin M. Ramasse[4], Andrew J. Morris[4], Jeremy Sloan[1], and David Quigley[1] — [1]University of Warwick, Coventry, UK — [2]University of Cambridge, Cambridge, UK — [3]Daresbury Campus, Darsbury, UK — [4]University of Birmingham, Birmingham, UK

We present the extreme case of nanostructuring, exploiting capillarity of single-walled carbon nanotubes (SWCNTs) for synthesis of the smallest possible thermoelectric SnTe nanowires with cross sections as small as a single atom. By adapting high-throughput ab initio random structure searching, we discover several structures of SnTe that can be formed within SWCNT and compare results with experimentally obtained encapsulated SnTe nanowires. From first principles, we demonstrate that by choosing the appropriate diameter of a template SWCNT, we can manipulate the structure of 1D SnTe and its thermoelectric performance. The demonstrated technique opens a practical route towards nanostructural manipulation of electrical and thermoelectric properties of the 1D materials. The best candidate 1D SnTe structures demonstrate strongly enhanced ZT over a unprecedentedly broad temperature range with a maximum value of 3.25.

O 118: Metal substrates: Structure, epitaxy and growth

Time: Friday 11:00–13:00 Location: MA 005

O 118.1 Fri 11:00 MA 005

Metal self-diffusion barriers on terraces and steps and their relation to dendrite growth in batteries — •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 serious safety and efficiency problem in batteries and can lead to short-circuits during battery operation. As metal growth processes are intimately linked to diffusion behaviour, we initially studied the self-diffusion properties of lithium, sodium and magnesium on the most stable surface terminations by first-principles electronic structure calculations [1]. We have now extended this study to the diffusion properties along and across steps and to other metals that are also used as charge carriers in batteries such as Zn and Al. Additionally, we have investigated the effect of the presence of electric fields on the terrace diffusion behaviour.

We argue that particularly the Ehrlich-Schwoebel barrier is relevant for the three-dimensional growth of metals and thus also dendrite growth. We will show that the new results confirm our previous considerations for Li and Mg. However, no consistent picture arises across all considered metals. Possible reasons for the inconsistencies will be discussed.

[1] M. Jäckle and A. Groß, J. Chem. Phys. **141**, 174710 (2014).

O 118.2 Fri 11:15 MA 005

Surface segregation and electromechanical coupling at the Ag-Au (111) surface — •Sandra Hoppe and Stefan Müller — Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

Recently, the sponge-like nanoporous gold (npAu) has attracted the attention for heterogeneous catalysis due to its promising characteristics, such as high catalytic activity at ambient temperature and pressure and a high surface-to-volume ratio[1]. Residual silver that is left after the fabrication process has been found to influence the catalytic activity and selectivity of npAu[2]. In order to better understand this phenomenon, it is crucial to analyze the way silver is distributed in the Ag-Au alloy surface and how segregation affects the surface composition. For this purpose, we have employed a combination of first-principles calculations and statistical physics to investigate surface segregation at the Ag-Au (111) surface. Interestingly, we obtain Au enrichment in the topmost layer, which we explain with a charge transfer from Ag to Au, stabilizing Au in the surface layer. Furthermore, we analyzed the influence of the surface composition and Ag surface concentration on the electromechanical coupling behavior, which offers an opportunity to alter the catalytic activity by applying strain to a surface.

[1] B. Zielasek *et al. Angew. chem. Int. Ed.* **45** (2006) 8241.
[2] L.-C. Wang *et al. Beilstein J. Nanotechnol.* **4** (2013) 111.

O 118.3 Fri 11:30 MA 005

(Meta)-stability of bimetallic surfaces: A computational study — •David Mahlberg and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The catalytic properties of bimetallic surfaces sensitively depend on their composition and/or structural arrangement. However, it is often not clear how stable these structures are under reaction conditions such as high temperatures. Here we present first principles-based kinetic Monte-Carlo (kMC) simulations to analyze the (meta-)stability of PtRu/Ru(0001) surface alloys.

Typically structural changes in metals occur via vacancy diffusion. In a first step, the enthalpy of vacancy formation was determined by density functional theory calculations. There is a high energetic cost of their formation, resulting in a small concentration of vacancies on the surface, in agreement with scanning tunneling microscope (STM) results [1]. In a second step, barriers for vacancy diffusion were derived as a function of the surrounding composition of bimetallic surface alloy which then enter the kMC simulations as jump rates derived via transition state theory. We will present results of the time evolution of the structure of PtRu/Ru(0001) surface alloys and analyze them in terms of the interaction between the constituents of the bimetallic surface.

[1] H. E. Hoster, A. Bergbreiter, P. M. Erne, T. Hager, H. Rauscher and R. J. Behm, Phys. Chem. Chem. Phys. **10**, 3812 (2008).

O 118.4 Fri 11:45 MA 005

X-ray standing wave excited photoemission experiments on W/C multilayer mirrors — •Marie Schmitz[1], Martina Müller[2], Ronja Anika Heinen[2], Patrick Lömker[2], Andrei Gloskovskii[3], Martina Müller[2], and Carsten Westphal[1] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany — [2]Forschungszentrum Jülich GmbH, PGI-6, Jülich, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

We report on the measurements of x-ray standing waves (XSW) generated on a bilayer system of alternating Carbon and Tungsten (W/C). The method of photo electron spectroscopy provides a high chemical sensitivity thus being element sensitive, without giving a spacial resolution. In contrast, X-ray reflection methods can provide this depth-resolution, without being element specific. The stated disadvantages can be overcome by using XSW-measurements as they both provide the advantages of these methods. In order to this, a thin periodic layer system of alternating refractive index materials has to be used to generate a strong standing wave while rocking the sample around the bragg angle. The multilayer including Si and Mo is a widely used system to generate standing waves on a surface. We use a W/C multilayer system, as it provides better temperature-stabilities, while keeping a high reflectance. In this context the reflectivity is an important figure of merit. The smoothness of the interface is a key property leading to a perfect interface without boundary imperfections.

O 118.5 Fri 12:00 MA 005

X-ray standing wave excited photoemission experiments on W/C multilayer mirrors — •Marie Schmitz[1], Philipp Espeter[1], Ronja Anika Heinen[2], Patrick Lömker[2], Andrei Gloskovskii[3], Wolfgang Drube[3], Martina Müller[2], and Carsten Westphal[1] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany — [2]Forschungszentrum Jülich GmbH, PGI-6, Jülich, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

The method of photoelectron spectroscopy provides a high chemical sensitivity thus being element sensitive, without giving a spacial resolution. In contrast, x-ray reflection methods can provide this depth-resolution, without being element specific. The stated disadvantages can be overcome by using XSW-measurements as they both provide the advantages of these methods. In order to this, a thin periodic layer system of alternating refractive index materials has to be used to generate a strong standing wave while rocking the sample around the bragg-angle. The multilayer including Si and Mo is a widely used system to generate standing waves on a surface. We use a bilayer system of alternating Carbon and Tungsten (W/C), as it provides better temperature-stabilities, while keeping a high reflectance. In this context the reflectivity is an important figure of merit. The smoothness of the interface is a key property leading to a perfect interface without boundary imperfections. We report on the measurements of x-ray standing waves (XSW) generated on a W/C multilayer system. A Pd cap was used as a test system.

O 118.6 Fri 12:15 MA 005

Temperature dependent growth of Zn and formation/decomposition of ZnO_x on Au(111) — •Konstantin M. Schüttler, Albert K. Engstfeld, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Methanol is a promising molecule for chemical energy storage, e.g., when using H_2 from renewable sources for its synthesis. Au/ZnO was found to be a highly active catalyst for the synthesis of "Green Methanol" from CO_2/H_2 as a "Solar Fuel"[1]. Previously, CuZn alloys have been used as model systems for the industrially used Cu/ZnO catalysts, for which it has been found that under reaction conditions ZnO at the perimeter of the Cu nanoparticles is partly reduced forming bimetallic CuZn sites[2]. For Au/ZnO this approach is similarly plausible. In order to gain more insight into the formation and nature of active sites, the formation, structure, electronic and chemical properties of bimetallic Zn/Au(111) surfaces serving as structurally well-defined 2D model catalysts were studied under UHV conditions. The temperature dependence of the nucleation, growth and alloy formation processes of Zn on Au(111) is discussed, based on STM studies. In addition, the reactivity of Zn surface atoms in the Au/Zn/O system, which may be crucial for the catalytic performance of ZnO supported MeOH synthesis catalysts, was studied by exposing Zn/Au(111) surfaces to molecular and atomic oxygen. Furthermore the deposition of Zn in an oxygen atmosphere and the thermal decomposition of these ZnO_x/Au(111) ($0 \leq x \leq 1$) surfaces has been studied.

O 118.7 Fri 12:30 MA 005

Energetics and structure of FeO/Fe(001) interfaces — •Tomasz Ossowski and Adam Kiejna — Institute of Experimental Physics, University of Wrocław, Pl. M. Borna 9, 50-204 Wrocław, Poland

The metal-oxide interfaces are of great importance in many fields of science and technology, including corrosion, catalysis, magnetic devices and spintronics. FeO thin layers on iron surfaces play significant role in growth of iron-oxides on the surfaces and in early stages of iron surfaces oxidation. In this work, we have performed DFT calculations of interaction of thin oxide films of 1-5 FeO atomic layers with Fe(001) surface. It is found that adsorption of single FeO layer on the Fe(001) surface results in a surface covered by oxygen atoms and subsequent oxide layers grow at the surface precovered by oxygen atoms. For thicker films of 2-5 FeO adlayers on Fe(001) surface, the system with oxygen atoms at the oxide-substrate interface is energetically most stable. The iron-oxide adsorption affects weakly substrate geometry causing expansion of the first interlayer distance compared to the clean iron surface. The work function of FeO/Fe(001) system is larger by about 0.2 eV than for the clean Fe(001) surface. The calculated work of separation shows that the strongest FeO-Fe(001) interactions occur for double FeO layers thick which is by about 0.45 eV stronger bound to Fe(001) surface than monolayer of FeO. For thicker FeO adlayers interaction weakens, however remains stronger than for the monolayer film. It is also found that FeO on Fe(001) surface exhibits antiferromagnetic order, with the interface layer oriented ferromagnetically to the substrate surface.

O 118.8 Fri 12:45 MA 005

Surface crystallography of large organic molecules on metal and insulator surfaces by LEED-IV using Fourier coefficients — •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

We will report on LEED-IV analysis of the large organic molecules PTCDA and NTCDA on the metal and insulator surfaces Ag(100), Ag(111), and KCl(100). Using data from different angles of electron incidence and optimizing the LEED-IV program code we were able to extend the experimental data set and shorten the calculation times required for the complex and large unit cells. Furthermore, the distortion of the PTCDA molecule and the buckling of the Ag surface were described by Fourier coefficients taking into account the symmetry of the system [1]. The idea of this procedure is to suppress unphysical vertical displacements of atoms on a short-wave-length scale by restriction to lower order coefficients.

By this, we obtain good Pendry R-factors, for PTCDA/Ag100 of about 0.23. We were able to derive the vertical distortions of the oxygen atoms in the functional group and the buckling of the Ag surface in rather good agreement with earlier results from DFT and NIXSW studies.

[1] W. Moritz et al, Phys. Rev. Lett. 104, 136102 (2010).

O 119: Non-Equilibrium Daynamics in Light-Driven Materials: Theory Meets Experiment

Time: Friday 11:30–13:00 Location: MA 141

O 119.1 Fri 11:30 MA 141

Long-lasting nonequilibrium in the electron system of laser-excited copper — •Sebastian T. Weber and Baerbel Rethfeld — Department of Physics and Research Center Optimas, University of Kaiserslautern, Erwin Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

After excitation with an ultra-short 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 ultra-fast laser excitation. Here, we focus on the study of copper which possesses a characteristic densities of states with an elevated area at a certain distance below the Fermi edge.

The results show the thermalization of the electrons towards Fermi distributions in a few femtoseconds. However, electron-phonon coupling hinders the electrons' complete thermalization as long as the quasi-temperatures of subsystems differ from each other. We present results showing these thermal and non-thermal non-equilibria and their timescales of relaxation.

O 119.2 Fri 11:45 MA 141

Relaxation of a laser-induced phonon nonequilibrium distribution — •Isabel Klett and Bärbel Rethfeld — Department of Physics and Optimas Research Center, University of Kaiserslautern, Germany

Femtosecond laser irradiation of solids leads to a thermodynamic nonequilibrium within and between the electron and phonon subsystems of the material. Due to collision processes, both subsystems relax into new thermodynamic equilibria within different respective thermalization times. In many studies, the nonequilibrium state within the phonon system is neglected and its influence on other relaxation processes is unclear. Here, we present a model for the description of the phonon nonequilibrium and its relaxation [1]. Phonon-phonon interactions are described with Boltzmann collision integrals. From this, an energy-dependent relaxation time can be extracted and inserted into a relaxation-time approach. Within the frame of this model, we study the thermalization of a nonequilibrium phonon distribution induced by ultrafast laser irradiation. It takes place on a timescale of some hundreds of femtoseconds. Additionally, we discuss the energy transfer between Fermi-distributed electrons and nonequilibrium phonons and compare this to the energy transfer between two equilibrated subsystems.

[1] I. Klett and B. Rethfeld, arXiv:1710.02355

O 119.3 Fri 12:00 MA 141

Hot phason dynamics in 1T-TaS2 probed by ultrafast LEED — •Theo Diekmann[1], Gerrit Horstmann[1], Simon Vogelgesang[1], Gero Storeck[1], Kai Rossnagel[2], and Claus Ropers[1] — [1]4th Physical Institute - Solids and Nanostructures, University of Göttingen, Friedrich-Hund-Platz 1, Germany — [2]Institute for Experimental and Applied Physics, University of Kiel, Germany

We recently developed an ultrafast low-energy electron diffraction (ULEED) setup for the time-resolved study of structural dynamics. To implement this approach in a backscattering geometry, a nanoscopic needle emitter is utilized in a miniaturized electrostatic lens geometry as a high-brightness photoelectron source [1]. In a first application, we investigated phase-ordering kinetics in the structural transition between CDW-phases in 1T-TaS2 [2].

Here, we study collective phase-excitations of the incommensurate CDW state, so-called phasons. By a comparison of the pump-induced intensity suppressions of Bragg- and CDW-satellite-reflections, we determine the time-dependent temperature changes in the respective subsystems. Our results reveal a strong initial energy transfer to the phason system, followed by a long-lived non-equilibrium between phasons and phonons, indicating an inhibited electron-phason relaxation channel. We attribute this observation to a gap-induced decoupling of electron and phason systems.

[1] G. Storeck et al., Structural Dynamics 4.4, 044024 (2017). [2] S. Vogelgesang et al., Nature Physics (2017), advance online publication.

O 119.4 Fri 12:15 MA 141

Photon-dressed states viewed by time- and angle-resolved photoemission spectroscopy — •Sven Aeschlimann[1], Mariana Chavez-Cervantes[1], Razvan Krause[1], Camilla Coletti[2], Kai Rossnagel[3], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany — [2]Center for Nanotechnology @ NEST, Istituto Italiano di Tecnologia, Pisa, Italy — [3]Institute of Experimental and Applied Physics, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

According to Floquet theory, the coherent interaction between Bloch states and strong photon fields generates side bands of the unperturbed band structure with the possibility to induce topological phase transitions when time reversal symmetry is broken with circularly polarized light[1]. The effect has been observed in Bi_2Se_3 using tr-ARPES[2]. There are predictions for related phase transitions in graphene[1] and transition metal dichalcogenides[3].

We present evidence for the generation of photon-dressed states in graphene and WSe_2 using tr-ARPES at extreme ultraviolet wavelengths. We discuss the key requirements for the experimental observation of these states, including the suppression of coherent interactions between the pump field and the photo-emitted electrons and a careful tuning of pump wavelength as well as pump and probe pulse durations.

[1] T. Oka and H. Aoki, PRB 79, 081406 (2009) [2] Y.H. Wang et al., Science 342, 453 (2013) [3] M. Claassen et al., Nature Communications 7, 13074 (2016)

O 119.5 Fri 12:30 MA 141

Light-induced femtosecond dynamics in C_{60}-films — •Razvan Krause, Mariana Chavez-Cervantes, Sven Aeschlimann, Andrea Cavalleri, and Isabella Gierz — Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany

Motivated by the recent discovery of a light-induced superconducting-like state in K_3C_{60} fullerides far above the critical temperature of 20 K [1] we are trying to unveil the underlying mechanism with time- and angle-resolved photoemission spectroscopy (tr-ARPES). We started by photo-exciting carriers across the HOMO-LUMO gap in C_{60} films grown on Si(111) with a resonant 1.5 eV femtosecond laser pulse, revealing an excited state life time of 50 fs. We are now exploring the possibility of driving large structural distortions of the C_{60} molecule through resonant excitation of the T_{1u} phonon mode at 7μm wavelength, which has been proposed to be responsible for the light-induced superconducting-like state in K_3C_{60} [1]. We present optical as well as tr-ARPES data that allow us to assess both the amplitude of the light-induced carbon displacements as well as the response of the electronic structure. We end by discussing the influence of doping and crystalline order for the light-induced C_{60} dynamics.

[1] Mitrano et al., Nature 530, 461 (2016)

O 119.6 Fri 12:45 MA 141

Ultrafast dynamics of bands and bonds in In/Si(111) nanowires probed by trARPES at 500 kHz — •Chris W. Nicholson[1], Andreas Lücke[2], Wolf Gero Schmidt[2], Michele Puppin[1], Laurenz Rettig[1], Ralph Ernstorfer[1], and Martin Wolf[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Universität Paderborn, Germany

In a Born-Oppenheimer description, nuclear dynamics evolve across a free energy surface determined by the occupation of electronic states as a function of nuclear coordinates. Ultrafast photo-induced phase transitions (PIPTs) provide a test case for how the forces and resulting nuclear motion along the reaction coordinate originate from a non-equilibrium population of excited electronic states.

Utilizing femtosecond time and angle resolved photoemission spectroscopy (trARPES) with a novel 500 kHz XUV laser source, we obtain direct access to the transient electronic structure during an ultrafast PIPT in a model system: the structural transition in In/Si(111) nanowires. A detailed reaction pathway is laid out, including temporally separated electronic and structural phase transitions. Comparison with ab initio molecular dynamics simulations reveals the crucial role played by localized photo-holes in shaping the potential energy landscape. Our detailed insights enable a combined momentum and real space description of ultrafast PIPTs including the ultrafast formation of chemical bonds [1].

[1] Nicholson et al. Submitted (2017)

O 120: Tribology: Surfaces and nanostructures

Time: Friday 11:30–13:00 Location: MA 144

O 120.1 Fri 11:30 MA 144

The Prandtl-Tomlinson model with time-varying interaction potential: Analytical predictions and experimental results — •Enrico Gnecco[1], Andre Schirmeisen[2], and Juan J. Mazo[3] — [1]Friedrich Schiller University Jena, Germany — [2]Justus Liebig University Giessen, Germany — [3]University of Zaragoza, Spain

The nonlinear Prandtl-Tomlinson (PT) model is possibly the simplest mechanism explaining the stick-slip motion of a sharp tip elastically pulled on a solid surface. In its basic version the PT model assumes uniform tip-surface interaction. Here we will assume that this is not the case and discuss the influence of contact oscillations and of a growing interaction strength due to "contact ageing" on the model results. In the former case the friction force is expected to decrease almost linearly with the oscillation amplitude until the stick-slip is replaced by steady sliding [1,2]. In the latter contact ageing results in a characteristic velocity weakening of friction which, in specific parameter ranges, can supersede the velocity strengthening caused by thermally activated stick-slip [3]. Interestingly, a similar approach can be used to reproduce the patterning process of compliant amorphous surfaces indented by a tip sliding on them [4]. The main predictions of the extended PT models are supported by experimental results on alkali halide and polymer surfaces in UHV and ambient conditions.

[1] R. Roth et al., App. Phys. Lett. 104, 083103 (2014). [2] O.Y. Fajardo et al., Phys. Rev. B 89, 075423 (2014). [3] J.J. Mazo et al., Phys. Rev. Lett. 118, 246101 (2017). [4] E. Gnecco et al., New J. Phys. 17, 032001 (2015).

O 120.2 Fri 11:45 MA 144

Temperature dependent Contact Ageing Dynamics of Silica Nano-Junctions — •Matthias Vorholzer[1], Guilherme Vilhena[2], Dirk Dietzel[1], Ruben Perez[2], Enrico Gnecco[3], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig-University, Giessen, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain — [3]Department for Mechanics of Functional Materials, Friedrich-Schiller-University, Jena, Germany

Contact ageing is a fundamental part of rate and state friction laws, which are commonly used to describe macroscale friction. Here, ageing is typically linked to changes of the contact area. Recent nanoscale experiments showed similar ageing for silica nano-junctions, but the effects were attributed to interfacial bond formation [1, 2]. Now, we are probing the temperature dependence of ageing to pinpoint further details about the intrinsic process. We present results for single-asperity slide-hold-slide [1] experiments under UHV conditions for temperatures ranging from 200 K to 300 K for a silica-silica interface. Key for our analysis is measuring the pre-rupture contact stiffness instead of static friction. Our results show logarithmic contact ageing at all temperatures with the expected temperature dependent slope. Additional

MD simulations were conducted, which show a striking agreement to the experiments, thereby confirming thermally activated formation of chemical bonds as the governing process for ageing.

[1] Q. Li et al., Nature 480, 233 (2011)

[2] K. Tian et al., PRL 118, 076103 (2017)

O 120.3 Fri 12:00 MA 144

Influence of phase transitions on nanoscale friction in the charge density wave material 1T-TaS$_2$ — Torben Marx[1], •Dirk Dietzel[1], Emanuele Panizon[2], Franco Pellegrini[2], Giuseppe E. Santoro[2,3,4], Erio Tosatti[2,3,4], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Giessen, Germany — [2]International School for Advanced Studies (SISSA), Trieste, Italy — [3]CNR-IOM Democritos National Laboratory, Trieste, Italy — [4]The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy

In recent years, analyzing the temperature dependence of nanoscale friction has proven to be an instructive tool to pinpoint internal relaxation modes for materials like polymers [1] or self-assembled monolayers (SAM) [2]. Now, we will show, that friction force microscopy can also be applied to characterize phase transitions by detecting the accompanying mechanical anomalies. To do so, the lateral force signal was constantly monitored during a continuous change of the sample temperature. As a model system, we analyzed the charge density wave material 1T-TaS2 and found, that e.g. the first order phase transition between the NC-CDW and the C-CDW phase was accompanied by distinct friction peaks. This behavior can be explained by a theoretical model, where small mechanical perturbations by the AFM tip are assumed to preemptively trigger the spinodal transformation, if the free energy barrier preventing this transformation becomes small enough.

[1] Jansen et al., PRL 102, 236101 (2009)

[2] Marx et al., Langmuir 33, 6005 (2017)

O 120.4 Fri 12:15 MA 144

Electrostatic Friction on Bi2Te3 (0001) — •Dilek Yildiz[1,2], Marcin Kisiel[1,2], Urs Gysin[1], Oguzhan Gürlü[3], and Ernst Meyer[1] — [1]Universität Basel, Basel, Switzerland — [2]Swiss Nanoscience Institute, Basel, Switzerland — [3]Istanbul Technical University, Department of Physics, Istanbul, Turkey

Bi2Te3 belonging into the class of topological insulators, has a bandgap in the bulk that makes the crystal semiconductor, whereas its surface is protected from backscattering. While protected topological systems are promising to observe exotic physical phenomena like Majorana fermion bounded state or magnetic monopoles, their frictional responses remain to be studied. Although in general 2D electronic systems are expected to strongly enhance the electrostatic friction, there is still lack of experimental evidence of it. Here we study electronic nature of Bi2Te3 surface and its effect on frictional response of the crystal by means of combined pendulum AFM/STM. While quantized image potential states which are above vacuum level were observed with STM, huge energy dissipation peaks were observed few nanometers above the surface with pendulum AFM. Energy dissipation peaks are localized at relatively large voltages as expected for image states and observed to be shifted to even higher voltages as tip-sample distance increase. Their relation was investigated in more detail by simultaneously operating STM and AFM. In this study, we observed that dissipation peaks are mainly due to electrostatic friction and closely related to image potential states.

O 120.5 Fri 12:30 MA 144

Pendulum AFM dissipation peaks and surface oxygen vacancies on SrTiO3 — Marcin Kisiel[1], Oleg Brovko[2], Dilek Yildiz[1], Remy Pawlak[1], Urs Gysin[1], Erio Tosatti[2], and •Ernst Meyer[1] — [1]Department of Physics, University of Basel,Klingelbergstr. 82, 4056 Basel, Switzerland — [2]International Centre for Theoretical Physics (ICTP), P.O.Box 586, I-34151 Trieste, Italy

Bodies in relative motion separated by few nanometer gap experiences a tiny friction force, whose nature is not understood. This non-contact form of friction can be successfully measured by highly sensitive cantilever oscillating like a tiny pendulum over the surface [1].

Recently it was reported that the critical fluctuations at the phase transition in a bulk SrTiO3 may affect the dissipation of mechanical probes even if completely external to the crystal surface [2]. Here we report on striking singlets or multiplets of dissipation peaks above SrTiO3 surface present at low temperatures (T=5K) and after sample annealing to high temperatures (T> 1000oC) which leads to oxygen deficient sample. The observed dissipation peaks are explained as arise due to a tip induced change of valency of the single quantum dot formed by oxygen vacancy (singlet), or groups of vacancies (multiplet). Moreover the results show strong dependence of dissipation peaks on the external magnetic field.

[1] - M. Kisiel et.al., Nature Materials10 (2011), 119-122. [2] - M. Kisiel,et.al., Phys. Rev. Lett.115 (2015), 046101.

O 120.6 Fri 12:45 MA 144

Friction at the Au/graphene interface: A density functional theory investigation — •Duygu Gizem Şentürk[1], Daniele Toffoli[2], and Hande Toffoli[1] — [1]Department of Physics, Middle East Technical University, 06800, Ankara, Turkey — [2]Dipartimento di Scienze Chimiche e Farmaceutiche, Universita degli Studi di Trieste, Via L. Giorgieri 1, I-34127, Trieste, Italy

As the confines of materials science extend to the nanoscale, the tribological behavior of materials diverges significantly from their macroscale counterparts as the classical Amontons-Coulomb laws no longer apply to interfaces since the quantum mechanical nature of the materials dominates. It is then of great importance to develop a new picture of friction at this scale, especially due to its increasing industrial importance. Friction Force Microscopy(FFM), has opened new frontiers in the study of these challenging interfaces. In particular, metal-coated tips have been used in FFM experiments to uncover the fascinating behavior of two-dimensional systems such as graphene, h-BN and MoS2. In this work, for the first time to the best of our knowledge, we will present a detailed density functional theory investigation of the direction-dependent friction forces that arise as a result of relative motion at the interface between graphene and low-index surfaces of Au. We will highlight the differences in the behavior of the (100), (110) and (111) surfaces and detail the results of our attempts to understand the source of these differences.This work is funded by The Scientific and Technological Research Council of Turkey (TUBITAK) within the 1001 program, Grant No: 115F493.

O 121: Overview Talk: Karsten Reuter

Time: Friday 13:15–14:00 Location: HE 101

Invited Talk O 121.1 Fri 13:15 HE 101

A look through the operando glass: First-principles based multiscale modeling of working catalysts — •Karsten Reuter — Technische Universität München

Increasingly available data from operando spectroscopies and microscopies point at a much more dynamic behavior of the surface of working catalysts than traditionally assumed. Instead of a catalytic function that is driven by static active sites as they emerge from a crystal lattice truncation of the nominal catalyst bulk material, a highly dynamic picture is suggested with continuous reaction-induced complex (surface) morphological changes at (near-)ambient reaction conditions or an evolving, possibly liquid-like phase behavior due to limited heat dissipation channels. Scrutinizing and complementing this insight through first-principles based modeling turns out to be a major challenge. The electronic structure level needs to be reliably described to maintain predictive quality. Mikrokinetic simulations have to account for the statistical interplay of all elementary processes, while macroscopic flow simulations evaluate the heat and mass transport in the non-ideal reactor geometries employed in the operando measurements. I will introduce corresponding advanced multiscale modeling approaches and discuss their current capabilities and limitations, using oxide formation in the context of oxidation catalysis as a showcase.