Surface Science Division
Fachverband Oberflächenphysik (O)

Axel Groß
Institut für Theoretische Chemie
Universität Ulm
Albert-Einstein-Allee 11
89069 Ulm
Axel.Gross@uni-ulm.de

Overview of Invited Talks and Sessions

(Lecture Rooms H15, H17, H31, H33, H36, H38, H42, and H45; Poster B1 and B2)

Invited Talks

O 1.1	Mon	9:30–10:15	H36	**Exciton fission, quantum coherence, & solar energy conversion beyond the limit** — •Xiaoyang Zhu
O 12.1	Mon	15:00–15:45	H36	**Interaction of Gas Phase Molecules with Nanostructured Model Supported Catalysts: Thermodynamics and Kinetics** — •Swetlana Schauermann
O 25.1	Tue	9:30–10:15	H36	**Flippable charge, magnetic, and orbital modulation at ferroelectric/manganite interfaces from first principles** — •Sohrab Ismail-Beigi
O 34.1	Tue	15:00–15:45	H36	**Ultrafast Spin and Magnetization Dynamics and their Signatures in the Transient Band Structure** — •Martin Weinelt
O 37.1	Wed	9:30–10:15	H36	**Single impurities in semiconductors studied by STM** — •Paul Koenraad
O 48.1	Wed	15:00–15:45	H36	**Surface-confined molecular nanoarchitectures: non-covalent and covalent construction and templated dynamics** — •Florian Klappenberger
O 59.1	Thu	9:30–10:15	H36	**Interatomic Potentials for Molecules, Solids, and Surfaces Based on Artificial Neural Networks** — •Jörg Behler
O 69.1	Thu	15:00–15:45	H36	**Electrocatalysis: from single crystals to single nanoparticles** — •Marc Koper
O 82.1	Fri	9:30–10:15	H36	**Plasmons, forces and currents in atomic and molecular contacts** — •Richard Berndt
O 92.1	Fri	13:15–14:00	H36	**Room-temperature electron spin filtering by ordered thin films of helical organic molecules** — •Helmut Zacharias

Topical Talks of the Focussed Session: Frontiers of electronic structure theory (jointly with HL and TT)

O 5.1	Mon	10:30–11:00	H36	**Fully ab initio determination of free energies: Basis for high-throughput approaches in materials design** — •Joerg Neugebauer, Fritz Kormann, Martin Friak, Blazej Grabowski, Timann Hickel
O 28.1	Tue	10:30–11:00	H36	**Materials for Alternative Energies: Computational Materials Discovery and Crystal Structure Prediction** — •Chris Wolverton
O 41.1	Wed	10:30–11:00	H36	**Challenges in data-intensive computational materials design: methodology and infrastructure.** — •Boris Kozinsky
O 51.1	Wed	16:00–16:30	H36	**Screening high throughput density functional theory calculations using simplified models.** — •Georg K. H. Madsen, Ingo Opahle, Alessandro Parma, Eunan J. McEniry, Ralf Drautz
O 62.1	Thu	10:30–11:00	H36	**Atomic-scale design of energy materials** — •Karsten W. Jacobsen

Topical Talks of the Focussed Session: Solid-liquid interfaces

O 64.1	Thu	10:30–11:00	H31	**Cooperative Phenomena at the Solid/Liquid Interface** — •Katharina Krischer
O 64.3	Thu	11:15–11:45	H31	**Electrochemical energy conversion - interesting challenges for Surface Scientists** — •Harry E. Hoster
O 64.5	Thu	12:15–12:45	H31	**Interaction of Pt-nanoparticles with graphitic carbon structures - a computational study** — •Alexander A. Auer, Wolfgang B. Schneider, Udo Benedikt
O 76.1	Thu	16:00–16:30	H31	**The origin of the high oxygen reduction activity on PtX (X= Sc, Y, La, Sm, Gd and ..) alloys and their activation mechanism.** — •Ib Chorkendorff
O 76.4	Thu	17:15–17:45	H31	**Coupling electrochemistry to an ICP-MS - online-investigation of electrode material dissolution** — •Karl Mayrhofer, Serhiy Cherevko, Angel Topalov, Anna Schuppert, Josef Meier, Aleksandar Zeradjanin, Ioannis Katsounaros

Gaede Prize Talk

O 47.1	Wed	13:15–13:55	H15	**Complex magnetic order on the atomic scale** — •Kirsten von Bergmann

Invited talks of the joint symposium SYQP: Quantum Plasmonics (jointly with HL, TT)

See SYQP for the full program of the symposium.

SYQP 1.1	Wed	15:00–15:30	H1	**Quantum plasmonics and applications in light harvesting** — •Peter Nordlander
SYQP 1.2	Wed	15:30–16:00	H1	**Deterministic quantum plasmonics with single nanodiamonds** — •Serge Huant, Oriane Mollet, Aurelien Cuche, Aurelien Drezet
SYQP 1.3	Wed	16:00–16:30	H1	**Optically-active hybrid nanostructures: Exciton-plasmon interaction, Fano effect, and plasmonic chirality** — •Alexander Govorov
SYQP 1.4	Wed	17:00–17:30	H1	**Quantum nano-optics: Interaction of metallic nano-particles with quantum emitters** — •Salvatore Savasta
SYQP 1.5	Wed	17:30–18:00	H1	**Non-dipolar & magnetic interactions with optical antennas** — Alberto Curto, Martin Kuttge, Marta Castro-López, Ion Hancu, Tim Taminiau, •Niek van Hulst

Invited talks of the joint symposium SYPM: Photons for Magnetism (jointly with MA, HL, MI)

See SYPM for the full program of the symposium.

SYPM 1.1	Thu	15:00–15:30	H1	**Ultrafast emergence of nanoscale ferromagnetism far from equilibrium** — •Hermann Dürr
SYPM 1.2	Thu	15:30–16:00	H1	**Free-Electron Laser for Ultrafast Measurements in Material Science** — •Sven Reiche
SYPM 1.3	Thu	16:00–16:30	H1	**Nanomagnetism seen by Femtosecond X-rays** — •Stefan Eisebitt
SYPM 1.4	Thu	16:30–17:00	H1	**Ultrashort Radiation Pulses at Storage Rings** — •Holger Huck
SYPM 1.5	Thu	17:00–17:30	H1	**Every atom counts - Magnetic properties of supported metal atoms and small alloy clusters** — Torben Beeck, Ivan Baev, Steffen Palutke, Kai Chen, Sören Meyer, Kari Jänkälä, Michael Martins, •Wilfried Wurth

Invited talks of the joint symposium SYES: Frontiers of electronic structure theory: Discovery of Novel Functional Materials (jointly with DS, HL, MA, MM, TT)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Molecular dynamics simulation of nucleation and growth of crystals from solution** — •Michele Parrinello

SYES 1.2	Fri	10:00–10:30	H1	**Describing, understanding, and discovering hybrid materials from first principles** — •Claudia Draxl
SYES 1.3	Fri	10:30–11:00	H1	**Mapping the Electronic Structure Landscape for Materials Discovery** — •Krishna Rajan
SYES 1.4	Fri	11:00–11:30	H1	**New ferroelectrics and antiferroelectrics by design** — •Karin Rabe
SYES 1.5	Fri	11:30–12:00	H1	**The Materials Project: The design of materials using high-throughput ab initio computations** — •Gerbrand Ceder

Sessions

O 1.1–1.1	Mon	9:30–10:15	H36	**Invited Talk (Xiaoyang Zhu)**
O 2.1–2.4	Mon	9:30–10:45	H10	**Topological Insulators 1 (jointly with DS, HL, MA, TT)**
O 3.1–3.7	Mon	9:30–11:15	H17	**Graphene: Magnetic Fields (jointly with DS, HL, MA, and TT)**
O 4.1–4.13	Mon	9:30–13:00	H20	**Transport: Quantum Dots, Wires, Point Contacts 1 (jointly with HL and TT)**
O 5.1–5.10	Mon	10:30–13:15	H36	**Focussed Session: Frontiers of Electronic Structure Theory I (jointly with HL and TT)**
O 6.1–6.10	Mon	10:30–13:00	H38	**Organic/bio Molecules on Metal Surfaces I**
O 7.1–7.10	Mon	10:30–13:00	H31	**Plasmonics and Nanooptics I**
O 8.1–8.11	Mon	10:30–13:15	H33	**Surface Chemical Reactions and Heterogeneous Catalysis I**
O 9.1–9.10	Mon	10:30–13:00	H42	**Nanotribology**
O 10.1–10.10	Mon	10:30–13:00	H45	**Nanostructures at Surfaces I**
O 11.1–11.9	Mon	11:30–13:45	H17	**Graphene: Spin-orbit interaction (jointly with DS, HL, MA, and TT)**
O 12.1–12.1	Mon	15:00–15:45	H36	**Invited Talk (Swetlana Schauermann)**
O 13.1–13.11	Mon	15:00–19:20	H2	**Focus Session: Crystalline n-type semiconducting oxides - SnO_2, Ga_2O_3, and In_2O_3 for novel devices (jointly with HL)**
O 14.1–14.10	Mon	15:00–18:00	H10	**Topological Insulators 2 (jointly with DS, HL, MA, TT)**
O 15.1–15.5	Mon	15:00–17:45	H20	**Focussed Session: Correlations in Topological Bands (jointly with DS, HL, MA, and TT)**
O 16.1–16.5	Mon	15:00–17:30	H23	**Magnetic Excitations: from surfaces down to adatoms (jointly with MA)**
O 17.1–17.13	Mon	16:00–19:15	H36	**Focussed Session: Frontiers of Electronic Structure Theory II (jointly with HL and TT)**
O 18.1–18.12	Mon	16:00–19:00	H38	**Organic/bio Molecules on Metal Surfaces II**
O 19.1–19.12	Mon	16:00–19:00	H31	**Plasmonics and Nanooptics II**
O 20.1–20.12	Mon	16:00–19:00	H33	**Surface Chemical Reactions and Heterogeneous Catalysis II**
O 21.1–21.11	Mon	16:00–18:45	H42	**Electronic Structure and Spin-Orbit Interaction I**
O 22.1–22.11	Mon	16:00–18:45	H45	**Nanostructures at Surfaces II**
O 23.1–23.12	Mon	16:00–19:00	H17	**Graphene: Electronic Properties and Transport (jointly with HL, MA and TT)**
O 24.1–24.6	Mon	17:15–18:45	H32	**Organic Electronics and Photovoltaics I (jointly with CPP, DS, HL)**
O 25.1–25.1	Tue	9:30–10:15	H36	**Invited Talk (Sohrab Ismail-Beigi)**
O 26.1–26.12	Tue	9:30–12:45	H17	**Transport: Graphene - Electronic Properties and Transport 2 (jointly with DS, HL, MA, and TT)**
O 27.1–27.12	Tue	9:30–12:45	H32	**Organic Electronics and Photovoltaics II (jointly with CPP, DS, HL)**
O 28.1–28.10	Tue	10:30–13:15	H36	**Focussed Session: Frontiers of Electronic Structure Theory III (jointly with HL and TT)**
O 29.1–29.11	Tue	10:30–13:15	H38	**Organic/bio Molecules on Metal Surfaces III**
O 30.1–30.10	Tue	10:30–13:00	H31	**Plasmonics and Nanooptics III**
O 31.1–31.11	Tue	10:30–13:15	H33	**Surface and Interface Magnetism I (jointly with MA)**
O 32.1–32.8	Tue	10:30–12:30	H42	**Metal Substrates I**
O 33.1–33.9	Tue	10:30–12:45	H45	**Nanostructures at Surfaces III**
O 34.1–34.1	Tue	15:00–15:45	H36	**Invited Talk (Martin Weinelt)**
O 35.1–35.91	Tue	18:15–21:45	Poster B1	**Poster Session I (Metal, semiconductor and oxide substrates: structure and adsorbates; Graphene)**

O 36.1–36.89	Tue	18:15–21:45	Poster B2	**Poster Session II (Organic films and electronics, photoorganics; Nanostructures; Plasmonics and nanooptics, Surface chemical reactions and heterogeneous catalysis, Surface dynamics)**
O 37.1–37.1	Wed	9:30–10:15	H36	**Invited Talk (Paul M. Koenraad)**
O 38.1–38.14	Wed	9:15–13:00	H16	**Topological Insulators (jointly with HL, MA, TT)**
O 39.1–39.13	Wed	9:30–13:00	H17	**Graphene: Characterization and Devices (jointly with DS, HL, MA, and TT)**
O 40.1–40.10	Wed	9:30–12:15	H23	**Spin Effects in Molecules at Surfaces (jointly with DS, MA)**
O 41.1–41.11	Wed	10:30–13:30	H36	**Focussed Session: Frontiers of Electronic Structure Theory IV (jointly with HL and TT)**
O 42.1–42.11	Wed	10:30–13:15	H38	**Organic/bio Molecules on Metal Surfaces IV**
O 43.1–43.11	Wed	10:30–13:15	H31	**Plasmonics and Nanooptics IV**
O 44.1–44.11	Wed	10:30–13:15	H33	**Scanning Probe Methods I**
O 45.1–45.9	Wed	10:30–12:45	H42	**Metal Substrates II**
O 46.1–46.8	Wed	10:30–12:30	H45	**Nanostructures and Clusters**
O 47.1–47.1	Wed	13:15–13:55	H15	**Gaede Prize Talk – Kirsten von Bergmann**
O 48.1–48.1	Wed	15:00–15:45	H36	**Invited Talk (Florian Klappenberger)**
O 49.1–49.5	Wed	15:00–18:05	H1	**Symposium Quantum Plasmonics (SYQP, jointly with HL, TT)**
O 50.1–50.6	Wed	15:00–18:00	H20	**Focussed Session: Majorana Fermions in Condensed Matter (jointly with DS, HL, MA, and TT)**
O 51.1–51.13	Wed	16:00–19:30	H36	**Focussed Session: Frontiers of Electronic Structure Theory V (jointly with HL and TT)**
O 52.1–52.12	Wed	16:00–19:00	H38	**Organic/bio Molecules on Metal Surfaces V**
O 53.1–53.13	Wed	16:00–19:15	H31	**Scanning Probe Methods II**
O 54.1–54.12	Wed	16:00–19:00	H33	**Organic Electronics and Photovoltaics (jointly with CPP, DS, HL)**
O 55.1–55.13	Wed	16:00–19:15	H42	**Electronic Structure and Spin-Orbit Interaction II**
O 56.1–56.12	Wed	16:00–19:00	H45	**Oxide Surfaces I**
O 57.1–57.13	Wed	16:00–19:15	H17	**Graphene: SiC Substrates and Intercalation (jointly with HL, MA and TT)**
O 58.1–58.87	Wed	18:15–21:45	Poster B1	**Poster Session III (Solid-liquid interfaces; Scanning probe and other methods; Electronic structure theory; Spin-orbit interaction)**
O 59.1–59.1	Thu	9:30–10:15	H36	**Invited Talk (Jörg Behler)**
O 60.1–60.9	Thu	9:30–13:30	H32	**Focussed Session: Organic Materials for Spintronics: From Spinterface to Devices (jointly with DS, HL, and MA)**
O 61.1–61.12	Thu	9:30–13:00	H34	**Organic Electronics and Photovoltaics I (jointly with CPP, DS, and HL)**
O 62.1–62.10	Thu	10:30–13:15	H36	**Focussed Session: Frontiers of Electronic Structure Theory VI (jointly with HL and TT)**
O 63.1–63.10	Thu	10:30–13:00	H38	**Plasmonics and Nanooptics V**
O 64.1–64.6	Thu	10:30–13:00	H31	**Focussed Session: Solid-liquid Interfaces I**
O 65.1–65.10	Thu	10:30–13:00	H33	**Surface and Interface Magnetism II (jointly with MA)**
O 66.1–66.11	Thu	10:30–13:15	H42	**Oxide Surfaces II**
O 67.1–67.5	Thu	10:30–13:00	H45	**Competition for the Gerhard Ertl Young Investigator Award**
O 68.1–68.11	Thu	10:30–13:15	H17	**Graphene: Preparation and Characterization I (jointly with HL, MA and TT)**
O 69.1–69.1	Thu	15:00–15:45	H36	**Invited Talk (Marc Koper)**
O 70.1–70.5	Thu	15:00–17:30	H1	**Symposium Photons in Magnetism (SYPM, jointly with MA, HL, MI)**
O 71.1–71.13	Thu	15:00–18:45	H3	**Surface Magnetism (jointly with MA)**
O 72.1–72.9	Thu	15:00–17:30	H17	**Graphene: Theory (jointly with DS, HL, MA, and TT)**
O 73.1–73.13	Thu	15:00–18:45	H34	**Organic Electronics and Photovoltaics II (jointly with CPP, DS, and HL)**
O 74.1–74.12	Thu	16:00–19:00	H36	**Focussed Session: Frontiers of Electronic Structure Theory VII (jointly with HL and TT)**
O 75.1–75.13	Thu	16:00–19:15	H38	**Organic/bio Molecules on Metal Surfaces VI**
O 76.1–76.9	Thu	16:00–19:00	H31	**Focussed Session: Solid-liquid Interfaces II**
O 77.1–77.13	Thu	16:00–19:15	H33	**Electronic Structure and Spin-Orbit Interaction III**

O 78.1–78.13	Thu	16:00–19:15	H42	**Surface Dynamics I**
O 79.1–79.10	Thu	16:00–18:30	H45	**Oxide Surfaces III**
O 80	Thu	19:30–20:00	H36	**Annual General Meeting of the Surface Science Division**
O 81	Thu	20:00–21:00	H36	**Post-Deadline Session**
O 82.1–82.1	Fri	9:30–10:15	H36	**Invited Talk (Richard Berndt)**
O 83.1–83.5	Fri	9:30–12:00	H1	**Symposium Frontiers of Electronic Structure Theory: Discovery of Novel Functional Materials (SYES, jointly with DS, HL, MA, MM and TT)**
O 84.1–84.17	Fri	9:15–13:45	H2	**Photovoltaics (jointly with CPP, DS and HL)**
O 85.1–85.13	Fri	9:30–13:00	H18	**Transport: Topological Insulators (jointly with DS, HL, MA, and TT)**
O 86.1–86.10	Fri	10:30–13:00	H36	**Plasmonics and Nanooptics VI**
O 87.1–87.10	Fri	10:30–13:00	H31	**Focussed Session: Solid-liquid Interfaces III**
O 88.1–88.9	Fri	10:30–12:45	H38	**Molecular Films**
O 89.1–89.11	Fri	10:30–13:15	H33	**Surface Dynamics II**
O 90.1–90.11	Fri	10:30–13:15	H45	**Semiconductor Substrates**
O 91.1–91.10	Fri	10:30–13:00	H17	**Graphene: Preparation and Characterization II (jointly with HL, MA and TT)**
O 92.1–92.1	Fri	13:15–14:00	H36	**Invited Talk (Helmut Zacharias)**

Annual General Meeting of the Surface Science Division

Thursday 19:30–20:00 H36

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

Post Deadline Session

Thursday 20:00–21:00 H36

Post Deadline Session followed by the Surface Science get-together.

O 1: Invited Talk (Xiaoyang Zhu)

Time: Monday 9:30–10:15 Location: H36

Invited Talk O 1.1 Mon 9:30 H36

Exciton fission, quantum coherence, & solar energy conversion beyond the limit — •Xiaoyang Zhu — Columbia University, USA

The maximum solar-to-electric power conversion efficiency of a conventional solar cell is determined by the Shockley-Queisser limit of ~31% [1]. A major reason for energy loss is because the absorption of photons with energy exceeding the bandgap creates hot electrons and holes with excess kinetic energy, which is quickly lost before the electrons and holes are captured. In this lecture, I will discuss a viable approach to exceed the Shockley-Queisser limit. This approach is based on the creation of two electron-hole pairs from the absorption of one photon in a process called singlet fission. I will illustrate how singlet exciton fission can occur in organic semiconductors due to a many electron quantum coherent process, and how to efficiently extract two electrons from the quantum coherent state [2-4]. These discoveries take us one step closer to designing solar cells with power conversion efficiency potentially exceeding the Shockley-Queisser limit.

[1] W. Shockley, H. J. Queisser, J. Appl. Phys. 32 (1961) 510-519.

[2] W.-L. Chan, M. Ligges, A. Jailaubekov, L. Kaake, L. Miaja-Avila, X.-Y. Zhu, Science 334 (2011) 1541.

[3] W.-L. Chan, M. Ligges, X.-Y. Zhu, Nature Chem. 4 (2012) 840-845.

[4] W.-L. Chan, J. R. Tritsch, X.-Y. Zhu, J. Am. Chem. Soc. 134 (2012) 18295-18302.

O 2: Topological Insulators 1 (jointly with DS, HL, MA, TT)

Time: Monday 9:30–10:45 Location: H10

Invited Talk O 2.1 Mon 9:30 H10

Breaking time reversal symmetry in topological insulators — •Jagadeesh Moodera — Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Breaking time reversal symmetry in a topological insulator (TI) can lead to many exotic properties, such as image magnetic monopole, topological magneto-electric effects as well as Majorana Fermions in superconducting TIs (STI). Recently Gedik*s group in MIT demonstrated that manipulating the magnetic properties via ultrashort light pulses, selectively exciting the spin states of the surface state by exploiting its spin texture to induce a transient magnetic state. Using linearly polarized light in a pump-probe experiment unusual behavior was seen by Muenzenberg group in Gottingen University. The TI surface state can be magnetically manipulated by proximity effect. The proximity-induced ferromagnetism in a TI/ferromagnetic insulator heterostructure breaks the time reversal symmetry in the TI: a large uniformly induced surface exchange gap appears on the TI without introducing scattering centers, thus keeping intact the transport of spin-momentum locked surface electrons as well as the superconducting pairing in an STI. This TI/ferromagnetic insulator bilayer system showed an induced interface magnetic moment accompanied by an unusual planar hysteresis magnetoresistance demonstrating the magnetic manipulation of the surface channel. This research is supported by ONR, NSF.

O 2.2 Mon 10:00 H10

Magnetic properties of the Mn doped topological insulator Bi$_2$Te$_3$ probed by ESR — •S. Zimmermann[1], V. Kataev[1], Huiwen Ji[2], R.J. Cava[2], and B. Büchner[1] — [1]IFW Dresden, 01171 Dresden, Germany — [2]Dept. Chem., Princeton Univ., NJ 08544, USA

Doping of a topological insulator (TI) with magnetic elements can break the time reversal symmetry and thus open a gap in the protected spin polarized conducting surface states, driving the system into a quantum spin Hall regime [1]. Understanding of the interactions between localized magnetic moments of dopants via delocalized electrons that give rise to ferromagnetism in TIs is therefore of significant interest. Such interactions can be of a long-range character and can also be mediated by surface conducting states [2]. Electron Spin Resonance (ESR) spectroscopy is a sensitive local technique that can probe interactions of localized spins with conduction electrons as well as spin-spin interactions in semiconductors and metals. In this contribution we report an ESR study of the Mn spin dynamics and magnetic interactions in high-quality single crystals of the Mn doped 3-dimensional TI Bi$_2$Te$_3$ [3]. We have observed a well-defined ESR signal from Mn spins and have studied the temperature dependences of the ESR parameters for a set of Bi$_2$Te$_3$ crystals with different Mn doping levels. The experimental ESR data will be presented in detail and the doping dependence of the Mn spin relaxation via conducting states and the establishment of ferromagnetic order as seen by ESR will be discussed. [1] R. Yu et al., Science **369**, 61 (2010); [2] L.A. Wray et al., Nature Physics **7**, 32 (2011); [3] Y.S. Hor et al., PRB **81**, 195203 (2010)

O 2.3 Mon 10:15 H10

Investigation of the relation between surface band gaps and magnetism in the magnetic topological insulator (Bi$_{1-x}$Mn$_x$)$_2$Se$_3$ — •Jaime Sánchez-Barriga[1], Andrei Varykhalov[1], Gunther Springholz[2], Hubert Steiner[2], Raimund Kirchschlager[2], Günther Bauer[2], Ondrei Caha[3], Enrico Schierle[1], Eugen Weschke[1], Akin Ünal[1], Sergio Valencia[1], Florian Kronast[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Johannes Kepler Universität Linz — [3]Masaryk University, Brno

The Dirac cone at the surface of a magnetic topological insulator is expected to open a band gap when ferromagnetically magnetized perpendicularly to the surface plane. Angle-resolved photoemission from epitaxial films of (Bi$_{1-x}$Mn$_x$)$_2$Se$_3$ shows for $x > 0.02$ a band gap at the Dirac point of a size that varies with Mn concentration, is much larger than theoretically predicted ($\sim$ 100 meV), and does not change with temperature from 7 to 300 K. Based on our measurements with x-ray magnetic circular dichroism (XMCD) we can exclude that the surface band gap is due to ferromagnetic order in the bulk or at the surface. In addition, we investigate by XMCD in photoemission microscopy the reported proximity magnetization induced by a ferromagnetic overlayer.

O 2.4 Mon 10:30 H10

Mapping the influence of cobalt atoms on the topological states of Bi2Te3 — •Paolo Sessi, Thomas Bathon, Lydia El-Kareh, and Matthias Bode — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg

Topological insulators are characterized by linearly dispersing gapless topological surface states protected by time-reversal symmetry. For these states, spin is perpendicularly locked to its momentum by spin-orbit interaction resulting in a chiral spin structure that forbids backscattering. However, this is predicted to not be the case when magnetic impurities are introduced into the system. Here, by means of scanning tunneling microscopy we investigate the robustness of the surface states of Bi2Te3 when single Co atoms are deposited on the surface. By analyzing the energy dependence of the quasi particle interference pattern produced by coherent scattering of surface states, we will examine the influence of Co atoms on scattering channels and energy dispersion relation.

O 3: Graphene: Magnetic Fields (jointly with DS, HL, MA, and TT)

Time: Monday 9:30–11:15 Location: H17

O 3.1 Mon 9:30 H17

Quantum interference in an electron-hole graphene ring system — •Dmitri Smirnov, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2 30167 Hannover, Germany

We analyze the electronic properties of a topgated monolayer graphene ring. Micro-mechanical cleavage was used to place a flake on a Si/SiO2 substrate. The structuring and contacting was done via plasma etching and electron beam lithography. An additional gate was placed on top of one arm of the ring which allows us to control the charge carrier concentration locally and additionally to create a pnp- (npn-) junction inside the ring. The sample was measured in a He3 cryostat and is identified as single layer graphene via magnetotransport measurements.

We observe Aharonov Bohm (AB) effect by sweeping the magnetic field around 0 T. The period of the oscillations is approx. 16 mT which fits the size of the ring well. The AB-oscillations are measured for different temperatures and the amplitude shows a saturation for lower temperatures. We also observe the AB-oscillations when a pnp-junction is created inside the ring. The period is independent of the existence of a pnp-junction and stays constant in all situations. We analyze the amplitude in dependence of the charge carrier concentration. The absolute amplitude is constant in the bipolar and unipolar region [1].

[1] D.Smirnov. et. al, Appl. Phys. Lett. 100, 203114 (2012).

O 3.2 Mon 9:45 H17

Experiments on Superlattice Graphene Structures with Patterned Top Gates — •Franz-Xaver Schrettenbrunner, Martin Drienovsky, Bastian Birkner, Sebastian Ringer, Dominik Koch, Dieter Weiss, and Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

We report on fabrication, finite element modelling (FEM), and the measurements of single- and bilayer graphene with structured top gates. By using micromechanically exfoliated graphene on SiO$_2$ surface, a Al$_2$O$_3$ dielectric was fabricated on top of the structure by either atomic layer deposition (ALD), evaporating thin aluminum films, or by combination of both methods. A digitated, patterned top gate electrode out of an AuPd alloy was fabricated by electron beam lithography (EBL). FEM yields that form and strength of the modulation strongly depend on thickness of the top gate dielectric, periodicity of the gate fingers, and applied voltage. Using both, the planar SiO$_2$ back gate and the patterned Al$_2$O$_3$ top gate the electric field effect creates variable modulations of the charge carrier concentration like pnp, nn'n, n0n, etc. along the whole underlying graphene. Measurements on these structures show typical behaviour for Klein-Tunneling resulting in an asymmetric curve of the Dirac Point. At high magnetic fields up to 14T unusual plateaus were observed when filling factors are mixing up in the top gated and the non top gated areas of the graphene samples.

O 3.3 Mon 10:00 H17

Weak Localization and Raman Study of Graphene Antidot Lattices Obtained by Crystallographically Anisotropic Etching — •Florian Oberhuber, Stefan Blien, Stefanie Heydrich, Tobias Korn, Christian Schüller, Dieter Weiss, and Jonathan Eroms — Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

We report the crystallographically anisotropic etching of exfoliated graphene on SiO$_2$ substrates by applying an etching mechanism that was demonstrated to eliminate carbon atoms located on armchair sites thus leading to zigzag edges [1]. Before exposing samples to this carbothermal reaction, they were patterned with circular antidots (diameter $\approx$40nm) by EBL and RIE. In the subsequent carbothermal etching step the predefined holes evolved into hexagonal antidots ($\approx$100nm).

We investigated a set of samples patterned with square lattices of hexagonal antidots and compare them to graphene patterned with lattices of circular holes investigated previously [2]. First, we compare samples by analyzing the weak localization peak in electron transport from which we obtain the phase coherence length and lengths for inter- and intravalley scattering. Second, samples were characterized by Raman spectroscopy focusing on G, D and D* peaks. In addition to the above mentioned comparison we demonstrate the influence of the etching reaction on graphene's properties by showing a series of Raman maps acquired between consecutive sample preparation steps.

[1] Nemes-Incze et al., Nano Res. (2010)

[2] Eroms et al., New J. Phys. (2009), Heydrich et al., APL (2010)

O 3.4 Mon 10:15 H17

Electronic structure of graphene twist flakes — •Wolfgang Landgraf, Sam Shallcross, Karla Türschmann, Dominik Weckbecker, and Oleg Pankratov — Lehrstuhl für Theoretische Festkörperphysik, Staudtstraße 7, D-91058 Erlangen

We study the electronic structure of bilayer graphene flakes with mutually rotated layers. The twist induces a large scale superstructure, a so called moiré pattern, which is a regular array of AA and AB stacked regions. We find that at low energies the electrons are trapped in the AA regions. This feature is visible even for a flake hosting a single AA moiré spot, which is thus acting as a quantum well. The electron density fluctuations induced by the moiré lattice are significant, being an order of magnitude greater than those generated by the rippling of a suspended graphene sheet. Finally, we determine the electronic properties of the twisted graphene flakes in the presence of an external magnetic field. We find a novel "zero-mode" structure, as well as Landau states that exhibit an electron current circulating between two graphene layers of the flake. The current distribution can be visualized as an electron flow on a torus circumventing the AA spot of the moiré lattice.

O 3.5 Mon 10:30 H17

Functionalized Graphene in Quantizing Magnetic Field: The case of bunched impurities — •Peter Silvestrov — Dahlem Center for Complex Quantum Systems, Freie Universitaet Berlin, 14195 Berlin, Germany

Covalent bonding of impurity atoms to graphene, in many cases leads to creation of unusual (singular) zero energy localized electron states. Existence of such states would lead to interesting phenomena, actively discussed recently.

In this talk I consider the behavior of localized impurity levels in graphene in quantizing magnetic field. In the magnetic field the impurity level effectively hybridizes with one of the n=0 Landau level states and splits into two close opposite-energy states. In turn, mixing of localized and Landau levels changes a spin content of a quantum Hall ferromagnet and modifies, via the exchange interaction, the spectrum of electrons surrounding the impurity.

Existing theories investigate graphene uniformly covered by adatoms, though some experiments indicate the tendency towards their clusterization. To address this ”unpleasant” possibility, I consider the case of a dense bunch of the impurity atoms, and show how such bunch changes dynamics and spin polarization of a large dense electron droplet surrounding it.

O 3.6 Mon 10:45 H17

Quantum Hall measurements on epitaxial graphene with oxygen adsorption — •Emiliano Pallecchi[1], Mohamed Ridene[1], Dimitris Kazazis[1], Felicien Schopfer[2], Wilfrid Poirier[2], Mark Goergig[3], and Abdelkarim Ouerghi[1] — [1]Laboratoire de Photonique et de Nanostructures (LPN-CNRS), 91460 Marcoussis, France — [2]Laboratoire National de Métrologie et d'Essais, 78197 Trappes — [3]Laboratoire des Physique de Solides, F-91505, Orsay

In this contribution we present quantum transport, ARPES, and LEED investigations of molecular oxygen-adsorbed epitaxial graphene grown on SiC. We show that the carrier concentration can be significantly reduced by exposing the sample to molecular oxygen. From Hall measurements we obtain a carrier concentration on the order of 1.2 x 10^{12} cm^{-2}, about one order of magnitude smaller than typical values of intrinsic epitaxial graphene. The reduction of electron doping is consistent with estimates from ARPES measurements. At high magnetic field, we find a fully developed quantum Hall effect, with a plateau at filling factor around 2, and a vanishing longitudinal resistance. Such a plateau is the hallmark of single layer graphene and suggests that the buffer layer is not fully decoupled from the substrate. This is further confirmed by LEED study. We then discuss the intermediate field regime, where we analyze the transition between a localized state observed at low fields and the quantum Hall regime at high fields. Finally, we compare these findings to the results obtained on epitaxial graphene exposed to atomic oxygen. We find that atomic oxygen is a more violent process that can damage significantly the graphene flake.

O 3.7 Mon 11:00 H17

Splitting of the Zero-Energy Landau Level and Universal Dissipative Conductivity at Critical Points in Graphene — •Frank Ortmann[1] and Stephan Roche[1,2] — [1]Catalan Institute of Nanotechnology, Barcelona (Spain) — [2]ICREA, Barcelona (Spain)

In graphene, the interaction of electrons with disorder impacts on their transport signature in a variety of experiments. Magnetotransport experiments can serve as an additional tool to probe this interaction with magnetic fields ranging from the low-field limit of weak antilocalization (∼mT) [1,2] to high fields defining the quantum Hall regime (∼10T). Being under study ever since the discovery of graphene, magnetic fields may unveil some interesting physics hidden otherwise or may generate new effects [3]. We are calculating the Kubo conductivity of graphene σ_{xx} and σ_{xy} in the presence of both weak and strong disorder and magnetic fields using a linear scaling method. This allows us to model realistic graphene samples up to micrometer size. Here we present our recent work on charge transport in the quantum-Hall regime and discuss our findings of universal conductivities. Particular emphasize is put on the non-trivial interference of disorder and magnetic-field and results from our novel order-N Hall-transport code.

[1] F.V. Tikhonenko et al. Phys. Rev. Lett. 103, 226801 (2009)
[2] F. Ortmann et al. EPL 94, 47006 (2011)
[3] D.A. Abanin et al. Science 332, 328 (2011)

O 4: Transport: Quantum Dots, Wires, Point Contacts 1 (jointly with HL and TT)

Time: Monday 9:30–13:00 Location: H20

O 4.1 Mon 9:30 H20

Tunneling-induced renormalization in interacting quantum dots — •Janine Splettstoesser[1], Michele Governale[2], and Jürgen König[3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University — [2]School of Physical and Chemical Sciences, Victoria University of Wellington, New Zealand — [3]Theoretische Physik, Universität Duisburg-Essen, Germany

A single-level quantum dot with arbitrarily strong onsite Coulomb interaction weakly coupled to electronic reservoirs is studied. We here present an analysis of tunneling-induced quantum fluctuations, generating cotunneling processes and renormalizing system parameters. For a perturbative treatment of these quantum fluctuations in the limit of weak tunnel coupling, we remove off-shell parts of the Hamiltonian via a canonical transformation. We find that the tunnel couplings for the transitions connecting empty and single occupation respectively single and double occupation of the dot renormalize with the same magnitude but with *opposite* signs [1]. This has an important impact on the shape of the renormalization extracted for example from the conductance. Finally, we verify the compatibility of our results with a systematic second-order perturbation expansion of the linear conductance performed within a diagrammatic real-time approach.

[1] J. Splettstoesser, M. Governale, J. König, Phys. Rev. B **86**, 035432 (2012).

O 4.2 Mon 9:45 H20

Interaction-induced charge and spin pumping through a quantum dot at finite bias — Hernan L. Calvo[1], •Laura Classen[1], Janine Splettstoesser[1], and Maarten R. Wegewijs[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany and JARA - Fundamentals of Future Information Technology — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

We discuss charge and spin transport through an adiabatically driven, strongly interacting quantum dot weakly coupled to two metallic contacts with finite bias voltage. We identify coefficients of response to the time-dependent external driving and relate these to the concept of emissivity [1]. These coefficients allow for a straightforward analysis of the predicted interaction-induced pumping under periodic modulation of the gate and bias voltage [2]. We extend this adiabatic Coulomb blockade spectroscopy to spin pumping. In the absence of a magnetic field, we show a striking, simple relation between the pumped charge at zero bias and at bias equal to the Coulomb charging energy. At finite magnetic field, we discuss the possibility to have interaction-induced pure spin pumping. For large-amplitude driving, the magnitude of both the pumped charge and spin saturates at values which are independent of the specific shape of the pumping cycle. Each of these values provides an independent, quantitative measurement of the junction asymmetry.

[1] M. Büttiker, H. Thomas, and A. Prêtre, Z. Phys. B 94, 133 (1994).
[2] F. Reckermann, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. Lett. 104, 226803 (2010).

O 4.3 Mon 10:00 H20

Structure and conductance analysis of atomic-sized contacts — •Manuel Matt[1], Fabian Pauly[1], Juan Carlos Cuevas[2], and Peter Nielaba[1] — [1]University of Konstanz, Department of Physics, 78457 Konstanz, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

We study the conductance histograms of different metals such as Au and Al. Our theoretical approach combines molecular dynamics simulations of the stretching of atomic-sized wires with the non-equilibrium Green's function formalism based on the tight-binding modelling of the electronic system. As compared to pervious work [1,2], we consider substantially larger wires and explore different lattice orientations. The results show good agreement with experiments.

[1] M. Dreher, F. Pauly, J. Heurich, J. C. Cuevas, E. Scheer, and P. Nielaba, Phys. Rev. B 72, 075435 (2005)
[2] F. Pauly, M. Dreher, J. K. Viljas, M. Häfner, J. C. Cuevas, and P. Nielaba Phys. Rev. B 74, 235106 (2006)

O 4.4 Mon 10:15 H20

Transport through two interacting resonant levels connected by a Fermi sea — •Elena Canovi, Alexander Moreno, and Alejandro Muramatsu — Institut für Theoretische Physik III, Universität Stuttgart

We study transport at finite bias, i.e. beyond the linear regime, through two interacting resonant levels connected by a Fermi sea. Our results are obtained by means of time-dependent density matrix renormalization group. We find that at finite size both the current and the occupations of the interacting levels oscillate as a function of time. We determine the amplitude and period of such oscillations as a function of bias and extension of the Fermi sea. In particular, the occupations on the two dots oscillate with a relative phase which depends on the distance between the impurities and on the Fermi momentum of the Fermi sea, as expected for RKKY interactions. The approximant to the steady-state current displays oscillations as a function of the distance between the impurities. In the free case we find that it is affected by resonances. The latter can be understood by considering the transmission coefficient of one particle propagating freely in the system. We discuss finally the incidence of interaction on such a behavior.

O 4.5 Mon 10:30 H20

Magnon-driven quantum-dot heat engine — •Björn Sothmann and Markus Büttiker — Départment de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

Recently, thermoelectric effects have generated a lot of interest. In Ref. [1], transport through two capacitively coupled quantum dots in a three-terminal setup was investigated in the Coulomb-blockade regime. It was shown how such a device can convert a heat current into a directed charge current. This converter is optimal in the sense that it transfers one electron for every quantum of energy delivered by the hot dot and thus allows to reach Carnot efficiency. A generalization to systems with many transport channels was analyzed in Ref. [2].

Here, we discuss a new class of devices where a single-level quantum dot is coupled to two ferromagnetic electrodes as well as to a ferromagnetic insulator at different temperatures [3]. We demonstrate that the system can convert a magnon current into a pure electron spin current or a spin-polarized electron current depending on the magnetic configuration. We analyze the maximal output power as well as the efficiency and show that the tight-coupling limit where heat and charge currents are proportional to each other can be reached.

[1] R. Sánchez and M. Büttiker, Phys. Rev. B **83**, 085428 (2011).
[2] B. Sothmann, R. Sánchez, A. N. Jordan and M. Büttiker, Phys. Rev. B **85**, 205301 (2012).
[3] B. Sothmann and M. Büttiker, EPL **99**, 27001 (2012).

O 4.6 Mon 10:45 H20

Iterative summation of path integrals for nonequilibrium molecular quantum transport — Roland Huetzen[1], •Stephan Weiss[1,2], Michael Thorwart[3], and Reinhold Egger[1] — [1]Heinrich-Heine Universität Düsseldorf, Universitätsstr.1, 40225 Düsseldorf — [2]Universität Duisburg-Essen and CENIDE, 47048 Duisburg — [3]Universität Hamburg, Jungiusstr. 9, 20355 Hamburg

We formulate and apply a nonperturbative numerical approach to the nonequilibrium current, $I(V)$, through a voltage-biased molecular conductor. We focus on a single electronic level coupled to an unequilibrated vibration mode (Anderson-Holstein model), which can be mapped to an effective three-state problem. Performing an iterative summation of real-time path integral (ISPI) expressions, we accurately reproduce known analytical results in three different limits. We then study the crossover regime between those limits and show that the Franck-Condon blockade persists in the quantum-coherent low-temperature limit, with a nonequilibrium smearing of step features in the IV curve.

[1] S. Weiss, J. Eckel, M. Thorwart, and R. Egger, Phys. Rev. B **77**, 195316 (2008).
[2] R. Hützen, S. Weiss, M. Thorwart, and R. Egger, Phys. Rev. B **85**, 121408 (2012).

15 min. break

O 4.7 Mon 11:15 H20

Spin dynamics in nanoparticles near Stoner instability — •Philipp Stegmann[1], Björn Sothmann[2], Jürgen König[1], and Yuval Gefen[3] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland — [3]Dept. of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel

We analyse the spin dynamics of a nanoparticle close to the Stoner instability. The nanoparticle is weakly tunnel coupled to two ferromagnetic leads. By mapping to an effective Fokker-Planck description we identify two different types of dynamic behaviour (diffusion vs. drift), which are revealed by characteristic relaxation times and a Fano factor that oscillates as a function of an applied bias voltage. Finally, we propose biasing schemes to generate states with magnetic quadrupole moments that dominate over a negligible dipole moment.

O 4.8 Mon 11:30 H20

Nonlinear transport through interacting quantum dots with superconducting leads in the weak coupling regime — •Sascha Ratz and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We present a nonequilibrium real-time diagrammatic transport theory for the systematic investigation of the quasiparticle and Josephson currents through a hybrid superconductor-quantum dot system in the weak coupling regime. In details, our device consists of an interacting quantum dot coupled to two biased spin-singlet superconducting leads. To describe the transport dynamics, we derive a completely general equation of motion for the reduced density matrix including all the contributions of a perturbation expansion in the tunneling Hamiltonian. Within these investigations, already in fourth order we can identify the contributions of the nonlocal time evolution kernel to the quasiparticle and DC Josephson transport. To clarify the difference between quasiparticle cotunneling and phase-coherent two-particle Andreev tunneling in fourth order, we first choose a single-level Anderson impurity model for the interacting quantum dot. In particular, one can give a clear explanation for subgap features due to proximity effects, which are also important when we finally compare our theoretical results for a carbon nanotube quantum dot with experimental observations.

O 4.9 Mon 11:45 H20

Spindephasing and Coherent Control of an Ensemble of Quantum Dots — •Andre Jovchev and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

We present a numerical treatment of pump-and-probe experiments with an ensemble of singly charged quantum dots in a magnetic field. We examine the excitation of trions, which is part of an effective polarization mechanism for the spin of the residual electrons, precessing around the magnetic field vector. Inhomogeneities in the magnetic g-factor of different electrons lead to dephasing. The effect of the short pump pulses is described by a unitary operator in the subspace of a spin degenerated electron and trion. For the dynamics between the pulses we apply a Lindblad theory to describe the decoherence due to environmental effects and the hyperfine interaction of the electrons with surrounding nuclei. We study the polarization of the whole ensemble after the application of different pulse protocols, and give an explanation for the polarization of the nuclear spins, which can lead to a remarkably increase of dephasing times which were already seen in experiments.

O 4.10 Mon 12:00 H20

Adiabatic pumping in the quasi-one-dimensional triangle lattice — Michael Schulze[1], •Dario Bercioux[1], and Daniel F. Urban[2,3] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [3]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

We analyze the properties of the quasi-one-dimensional triangle lattice emphasizing the occurrence of flat bands and band touching via the tuning of the lattice hopping parameters and on-site energies [1]. The spectral properties of the infinite system will be compared with the transmission through a finite piece of the lattice with attached semi-infinite leads. Furthermore, we investigate the adiabatic pumping [2] properties of such a system: depending on the transmission through the lattice, this results in nonzero integer charge transfers or transfers that increase linearly with the lattice size.

[1] M. Schulze, D. Bercioux, D. F. Urban, arXiv:1208.6113.
[2] P. W. Brouwer, Phys. Rev. B **58**, 10135(R) (1998).

O 4.11 Mon 12:15 H20

Thermoelectric efficiency of a driven double quantum dot — •Federica Haupt[1], Stefan Juergens[1], Michael Moskalets[2], and Janine Splettstoesser[1] — [1]RWTH Aachen University, Aachen, Germany — [2]Kharkiv Polytechnical Institute, Kharkiv, Ukraine

By applying phase-shifted AC signals to the gates of two quantum dots connected in series, it is possible to transfer charge from one lead to another in a quantized way [1,2], even in the presence of an applied bias voltage or a temperature gradient. In this work we investigate the thermoelectric properties of such a double quantum dot device. We show that not only charge but also heat can be pumped in a quantized way. If the modulation frequency Ω is sufficiently small, we find regimes in which the unit of heat $2\pi k_B T \ln 2$ is transported during each period, where T is the temperature of the considered lead and the factor $\ln 2$ stems from spin degeneracy. This would open the possibility of using the pumping cycle to transfer heat against a temperature gradient or to extract work from a hot reservoir with Carnot efficiency. However, the performance of a real device is limited by dissipative effects due to leakage currents and finite time operation, which we rigorously take into account by means of a real-time diagrammatic approach in the regime of weak coupling to the leads. We show that despite these dissipative effects, efficiencies up to 70% of the maximal theoretical value can be reached.

[1] H. Pothier, *et al.*, Europhys. Lett **17**, 249 (1992)
[2] S. J. Chorley, *et al.* App. Phys. Lett. **100**, 143104 (2012).

O 4.12 Mon 12:30 H20

Controlling entanglement and spin-correlations in double quantum dots in the non-equilibrium regime — •Carlos Alberto Büsser[1] and Fabian Heidrich-Meisner[2] — [1]Ludwig-Maximilians-Universität, München, München — [2]FAU Erlangen-Nuremberg and LMU München

We study the non-equilibrium dynamics in a parallel double-quantum dot structure induced by a large bias voltage. By applying both a magnetic flux and a voltage, it is possible to generate spin-spin-correlations between the two quantum dots. The sign and absolute value of these correlations can be controlled by changing the bias voltage. Using a canonical transformation we argue that the mechanism that drives the spin-spin correlations can be understood in terms of an effective Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction that is mediated by the current. Our study is based on the Anderson-impurity model and we use time-dependent density matrix renormalization group (tDMRG) simulations to obtain currents and spin-correlations in the steady state of the non-equilibrium regime. We also perform quench in the Hamiltonian to prove the stability of the entangled state.

O 4.13 Mon 12:45 H20

Role of coherent state superpositions in the bipolar spin blockade of a triple quantum dot — Maria Busl[1], Ghislain Granger[2], Louis Gaudreau[2], •Rafael Sánchez[1], Alicia Kam[2], Michel Pioro-Ladrière[3], Sergei Studenikin[2], Piotr Zawadzki[2], Zbigniew Wasilewski[2], Andrew Sachrajda[2], and Gloria Platero[1] — [1]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain — [2]National Research Council Canada, Ottawa, Canada — [3]Université de Sherbrooke, Sherbrooke, Canada

In double quantum dots, Pauli spin blockade manifests as a rectified current: charge flows or is blocked depending on the sign of the applied voltage[1]. We present experimental and theoretical investigations of the equivalent process in triple quantum dots in series. We focus on a configuration where (2,0,2) (2,1,1), (1,1,2) and (2,1,2) states are degenerate. When a bias is applied in a magnetic field beyond 10mT, bipolar spin blockade is observed where current is suppressed independent of the applied bias direction. As the field is reduced to zero, leakage resonances are observed. Of special interest are two very sharp resonances which correspond to triple dot conditions when states in the left and right dot but not the center dot align. One of these resonances is found itself to involve bipolar spin blockade and is found to result from a purely quantum coherent effect: electrons occupy states that involve their transference from one extreme to the other of the triple quantum dot without ever visiting the center[2].

[1] K. Ono et al., Science 297, 1313 (2002).

[2] M. Busl et al., unpublished.

O 5: Focussed Session: Frontiers of Electronic Structure Theory I (jointly with HL and TT)

Organizers: R. Drautz (Ruhr-Universität Bochum), N. Marzari (EPFL, Lausanne), Matthias Scheffler (FHI, Berlin)

Time: Monday 10:30–13:15 Location: H36

Topical Talk O 5.1 Mon 10:30 H36

Fully ab initio determination of free energies: Basis for high-throughput approaches in materials design — •Joerg Neugebauer, Fritz Kormann, Martin Friak, Blazej Grabowski, and Timann Hickel — MPI für Eisenforschung, Düsseldorf, Germany

A key requirement in developing systematic tools to design novel materials on the computer is the availability of accurate computational tools determining energies not only at $T = 0$ K but also under realistic conditions, i.e., at finite temperature. Combining accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts allows now to address this issue and to determine free energies and derived thermodynamic quantities such as heat capacity, thermal expansion coefficients, and elastic constants with an accuracy that often rivals available experimental data.

In the talk we will show how novel sampling strategies in configuration space together with highly converged density-functional theory calculations allow an unbiased and accurate determination of all relevant temperature dependent free energy contributions. The flexibility and the predictive power of these approaches and the impact they can have in developing new strategies in materials design will be discussed for modern high strength steels and light weight metallic alloys.

O 5.2 Mon 11:00 H36

Fast screening of perovskites' phase stability using AIDA, a materials' informatics platform for materials design and discovery — •Giovanni Pizzi[1], Andrea Cepellotti[1], Boris Kozinsky[2], Marco Fornari[3], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, EPFL (CH) — [2]Robert Bosch LCC Research and Technology Center, Cambridge (USA) — [3]Dept. of Physics, Central Michigan University (USA)

Many perovskite systems display a high-temperature cubic phase with zero net polarization, whose microscopic nature is still debated. We perform a systematic study of this phase for representative ABO_3 perovskites, showing that there is not a unique microscopic model for it. Some systems are consistent with a displacive or an order/disorder model; others can sustain a stable displacement pattern of B-site cations in supercells, preserving zero net polarization. In such high-throughput searches, a key challenge is the need of a "materials' informatics" infrastructure to automatically prepare, execute and monitor workflows of calculations for large classes of materials, and then retrieve, store and analyze the results. To this aim, we are developing an open-source platform for high–throughput (AIDA–"Automated Infrastructure and Database for Ab-initio design"). Using AIDA free-energy workflows, we studied the phase stability of $BaTiO_3$, evaluating the critical temperatures between the cubic, tetragonal, orthorhombic, and rhombohedral phases.

O 5.3 Mon 11:15 H36

Fast ab-initio screening of magnetic properties applied to the design of new hard magnetic materials — •Nedko Drebov[1], Christian Elsässer[1], Lothar Kunz[2], Alberto Martinez[2], Takashi Shigematsu[3], and Thomas Eckl[2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]Robert Bosch GmbH, Stuttgart, Germany — [3]Bosch Corporation, Tokyo, Japan

We present a fast computational ab-initio screening method which we use for the identification of new permanent magnetic materials based on rare-earth (RE) and transition-metal (TM) elements.

The candidates for new hard magnetic phases with specific structures and compositions are selected from ab-initio screening of their magnetic properties by using the TB-LMTO-ASA method. This procedure considers a large variety of possible combinations of RE and TM elements. At rather low computational costs one can get sufficiently accurate magnetic moments and exchange coupling parameters to be subsequently used in the process of virtual material design.

The results for selected candidate phases are further refined with a more accurate ab-initio method without potential-shape approximation. The Curie temperatures of the phases can be estimated from the calculated magnetic moments and exchange coupling by means of Monte Carlo simulations.

Acknowledgement: This work was supported by the Co-Operative Project 'Suche nach neuen hartmagnetischen Phasen mit hoher Energiedichte (REleaMag)' funded by the BMBF.

O 5.4 Mon 11:30 H36

Designer Single-Band Hubbard Materials — •Sinead Griffin and Nicola Spaldin — ETH Zurich, Switzerland

The low-energy physics of the High-Tc superconducting cuprates is believed to be encompassed in a single-band Hubbard model. Much work focuses on the computational solutions of the Hubbard model with a view to understanding the complex nature of metal-insulator transitions, superconductivity and strong-correlations physics in general.

Here we take the opposite approach of designing a real material which has the Hamiltonian of a 'single-band Hubbard model' material using first-principles electronic structure theory. By combining crystal field splitting with chemistry, we engineer a class of candidate materials with a single d-electron band at the Fermi level. We report the results of ab initio calculations of the electronic and magnetic structure of these new designer materials and discuss the possibilities for experimental synthesis.

O 5.5 Mon 11:45 H36

The stability of Bi-Sb-Te layered structures: a first-principles study — •Kirsten Govaerts[1], Marcel H.F. Sluiter[2], Bart Partoens[3], and Dirk Lamoen[1] — [1]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium — [2]Department of Materials Science and Engineering, 3mE, Delft University of Technology, Mekelweg 2, 2628 CD, Delft, The Netherlands — [3]CMT group, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium

Using an effective one-dimensional cluster expansion in combination with first-principles electronic structure calculations we have studied the energetics and electronic properties of Bi-Sb-Te layered systems. Our modified, quintuple based cluster expansion explicitly accounts for the Bi and Sb bilayer formation which is due to a Peierls instability. With this new method, groundstates of Bi-Sb-Te can be found without making the dataset of ab initio calculated structures unreasonably large. Groundstates are found within the binary alloys X-Te, with X corresponding to Bi or Sb, for a Te concentration between 0 and 60 at.%. They form an almost continuous series of (meta)stable structures consisting of consecutive X bilayers next to consecutive X_2Te_3 units. Another binary groundstate is the BiSb structure, consisting of alternating Bi and Sb layers, again forming pairs. Groundstates of ternary compounds all consist of consecutive units of Bi_2Te_3, Sb_2Te_3 and TeSbTeBiTe.

O 5.6 Mon 12:00 H36

RPA Correlation Potential in the Adiabatic Connection Fluctuation-Dissipation formalism — •Stefano de Gironcoli[1], Nicola Colonna[1], and Ngoc Linh Nguyen[1,2] — [1]Scuola Internazionale Superiore di Studi Avanzati (SISSA), via Bonomea 265, I-34136 Trieste, Italy — [2]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH)

Calculations of correlation energies within the formally exact Adiabatic Connection Fluctuation-Dissipation (ACFD) formalism, within the Random Phase Approximation (RPA) for the exchange-correlation kernel, have been recently carried out for a number of isolated and condensed systems. The efficiency of such calculations has been greatly improved by exploiting iterative algorithms to diagonalize RPA dielectric matrices [1]. However for several systems correlation energies may significantly depend about the choice of input single particle wavefunctions [2]. We derive an expression for the RPA self-consistent potential based on Density Functional Perturbation theory and we present self-consistent RPA calculations for weakly bound molecular dimers, including the controversial case of Beryllium dimer. In this case the self-consistent determination of RPA potential is crucial to determine the stability of the system which however results to be unstable toward dissociation in separated fragments.

[1] H.-V. Nguyen and S. de Gironcoli, Phys. Rev. B 79, 205114 (2009); H. F. Wilson, F. Gygi, and G. Galli, Phys. Rev. B 78, 113303 (2008).

[2] Huy-Viet Nguyen and G.Galli, J. Chem.Phys. 132, 044109 (2010).

O 5.7 Mon 12:15 H36

The bond-breaking and bond-making puzzle: many-body perturbation versus density-functional theory — •F. Caruso[1], D. Rohr[2], M. Hellgren[3], X. Ren[1], P. Rinke[1], A. Rubio[4,1], and M. Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Rice University, Houston, USA — [3]SISSA, Trieste, Italy — [4]Universidad del Pais Vasco, Donostia, Spain

Diatomic molecules at dissociation provide a prototypical situation in which the ground-state cannot be described by a single Slater determinant. For the paradigmatic case of H_2-dissociation we compare state-of-the-art many-body perturbation theory in the *GW* approximation and density-functional theory (DFT) in the exact-exchange plus random-phase approximation for the correlation energy (RPA). Results from the recently developed renormalized second-order perturbation theory (rPT2) are also reported. For an unbiased comparison and to prevent spurious starting point effects both RPA and *GW* are iterated to *full* self-consistency (i.e. sc-RPA and sc-*GW*). Both include topologically identical diagrams for the exchange and correlation energy but are evaluated with a non-interacting Kohn-Sham and an interacting *GW* Green function, respectively. This has profound consequences for the kinetic and the correlation energy. *GW* and rPT2 are both accurate at equilibrium, but fail at dissociation, in contrast to sc-RPA. This failure demonstrates the need of including higher order correlation diagrams in sc-*GW*. Our results indicate that RPA-based DFT is a strong contender for a universally applicable electronic-structure theory. F. Caruso *et al.* arxiv.org/abs/1210.8300.

O 5.8 Mon 12:30 H36

Density-Functional Theory Applied to Rare Earth Metals: Approaches Based on the Random-Phase Approximation — •Marco Casadei[1], Xinguo Ren[1], Patrick Rinke[1], Angel Rubio[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]University of the Basque Country UPV/EHU, Donostia, Spain

The description of the volume collapse exhibited by some *rare earth* metals poses a great challenge to density-functional theory (DFT) since local/semilocal functionals (LDA/GGA) fail to produce the associated phase transitions. We approach this problem by treating all electrons at the same quantum mechanical level, using both hybrid functionals (e.g. PBE0 and HSE06) and exact-exchange plus correlation in the random-phase approximation (EX+cRPA). We also assess the performance of recently developed beyond RPA schemes (e.g. rPT2 [1]). The calculations are performed for cerium and praseodymium, that display a volume collapse, and neodymium, in which the volume collapse is absent. The isostructural α-γ phase transition in cerium is the most studied. The exact exchange contribution in PBE0 and HSE06 is crucial to produce two distinct solutions that can be associated with the α and γ phases, but quantitative agreement with the extrapolated phase diagram requires EX+cRPA [2]. [1] Ren *et al.*, J. Mater. Sci. **47**, 7447 (2012). [2] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

O 5.9 Mon 12:45 H36

Thermodynamics of the $\alpha \rightleftharpoons \gamma$ transition in cerium from first principles — •Jordan Bieder and Bernard Amadon — CEA, DAM, DIF, F-91297 Arpajon, France

The Dynamical Mean Field Theory (DMFT) combined with density functional theory has been successful to describe strongly correlated materials [1]. However, the computation of the ground state properties requires a good accuracy from both the DFT and the DMFT side. We use thus a strong coupling Continuous Time Quantum Monte Carlo (CT-QMC) solver, which is fast and able to reach low temperatures, in combination with a projector augmented wave (PAW) DMFT implementation.

Extensive calculations using this implementation allows us to carefully reassess the ground state properties and thermodynamics of the $\alpha \rightleftharpoons \gamma$ phase transition in Cerium at low temperatures. In particular, stochastic noise is small enough to avoid any ambiguity on the interpretation of energy versus volume curves. The DMFT picture is put in perspective with recent DFT calculations [2] and recent experimental investigations [3,4].

[1] G. Kotliar *et al.* Rev. Mod. Phys. 78, 865(2006)
[2] M. Casadei *et al.* Phys. Rev. Lett. 109, 146402(2012)
[3] F. Decremps *et al.* Phys. Rev. Lett. 106, 065701(2011)
[4] M. J. Lipp *et al.* Phys. Rev. Lett. 109, 195705 (2012)

O 5.10 Mon 13:00 H36

Exciton dispersion in wide-gap insulators: there and back again — •Francesco Sottile[1,2] and Matteo Gatti[1,2] — [1]LSI, Ecole Polytechnique, Palaiseau, France — [2]European Theoretical Spectroscopy Facility

We present ab initio calculations of exciton dispersion of wide-gap insulators, like LiF and solid Argon. With the help of the Bethe-Salpeter equation (recently extended to describe full coupling finite momentum excitonic effects) we calculate the momentum dispersion of the first low-lying excitons, both visible and dark. Their particular behaviour (the exciton shows up, lower down, shows up again, to finally disapper) is analized with respect to: direction of the momentum dispersion, the coupling effect, real space exciton distribution and many-body interference effects. The results [1] are finally compared with recent inelastic X-ray scattering experiments [2,3] for what concerns LiF, while they constitutes a completely ab initio prediction for solid Ar.

[1] The Bethe-Salpeter calculation are carried out with the EXC code (http://www.bethe-salpeter.org/) [2] P.Abbamonte et al., PNAS 105, 12159 (2008) [3] C.-C. Lee et al. arXiv:1205.4106v1

O 6: Organic/bio Molecules on Metal Surfaces I

Time: Monday 10:30–13:00 Location: H38

O 6.1 Mon 10:30 H38

adsorption structure of PbPc on the surface Ag(111) — •peng jiang and michael hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surface Analysis Group, D-09107 Chemnitz, Germany

We have investigated the adsorption of PbPc on Ag(111) surface. Using OMBE technology, ultrathin films of PbPc have been deposited on Ag(111) and annealed at 100°C for 20min. The ordered molecular arrangement is observed when the molecular film is close or more than one monolayer. We have found two different adsorption structures with molecular unit cells characterized by side lengths of 1.53nm*1.45nm and 1.61nm*1.37nm, and angles of 85° and 89° respectively. On Ag(111) surface we found the shuttle-cock shaped molecules are in both Pb -up and -down adsorption configurations forming the chessboard like pattern. The reversible flipping between molecular configurations on the surface recorded during the scanning process proposes a new mechanism to control the single-molecular adsorption configuration on Ag(111) surface. With a slightly thicker film the molecules on the second layer lie directly on top and have the same orientation of that from the first layer making a direct stack.

O 6.2 Mon 10:45 H38

LEEM investigation of the initial growth of hetero-organic layers — •Caroline Henneke, Benjamin Stadtmüller, Thomas Duden, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and Jülich Aachen Reseach Alliance (JARA)-Fundamentals of Future Information Technology

One crucial issue for the success of organic materials in electronic devices is the ability to specifically design the interfaces between different active layers according to their functional purpose. The initial growth, i.e., the formation of the first molecular layer, is of particular interest in this context as this layer acts as a template for further growth.

We recently started to investigated hetero-organic layers consisting of Copper-II-phthalocyanine (CuPc) and 3,4,9,10-perylentetracarboxylic-acid dianhydride (PTCDA) on Ag(111). Using LEEM/PEEM, LEED and STM, we have identified three mixed phases with different stoichiometry. Kinetic processes like thin film growth, the formation of the organic mixed layer, and the transition between different phases were studied in real time with LEEM. The lateral structure of the different phases was investigated with SPA-LEED and STM.

O 6.3 Mon 11:00 H38

Electronic coupling in hetero-organic structures on Ag(111) — •Benjamin Stadtmüller[1,2], Martin Willenbockel[1,2], Daniel Lüftner[3], Eva M. Reinisch[3], Christoph Schmitz[1,2], Sergey Soubatch[1,2], Michael G. Ramsey[3], Peter Puschnig[3], F. Stefan Tautz[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology — [3]Institut für Physik, Karl Franzens-Universität Graz, 8010 Graz, Austria

The performance of organic materials in electronic devices depends on the ability to control the properties at the interfaces between different active layers. While almost all studies up to now focused on organic layers containing only one molecular species, some groups have recently started to investigate hetero-organic films with two different types of molecules. We have chosen mixed monolayer structures of CuPc and PTCDA adsorbed on Ag(111) as a model system. Our structural data revealed different long range ordered structures depending on the relative coverage of CuPc to PTCDA. The influence of intermolecular interactions on the electronic structure was studied by angle resolved photoelectron spectroscopy (ARPES). Analyzing the ARPES data in the orbital tomography approach [1] indicated a significant change in the occupation of the molecular orbitals in the mixed films. These modifications are correlated to the formation of an interface state expanding over both molecular species which leads to a coupling of the molecular valence states. [1] P. Puschnig et al, PRB 84, 235427 (2011)

O 6.4 Mon 11:15 H38

Identification of two different charge transfer mechanisms at Phthalocyanines/Ag interfaces — •Eric Salomon and Thierry Angot — Aix-Marseille university, Marseille, France

As the performance of organic molecule based electronic devices depends critically on the electrode-organic interfaces it appears crucial to have thorough understanding of the fundamental processes governing the metal-molecule interactions.

The vibrational properties of several M-phthalocyanines (here with M=H2, Zn, Cu, Co, Fe) adsorbed on Ag surfaces have been carefully investigated using high resolution electron energy loss spectroscopy (HREELS). In the monolayer range, a wide loss feature ranging from 200 up to 800 meV is commonly observed that displays a positive quadratic dispersion. It is interpreted as a surface-plasmon resulting from a space-charge region arising from an electron-vibration coupling at the interface between the organic monolayer and the metallic substrate. Nevertheless, significant differences are observed depending on the metal atom M. In most cases, while Infra Red active modes dominate, some vibrational motions of the adsorbate are damped by energy transfer to the metal substrate leading to Raman active modes with Fano line shape. However, this is not the case for Co- and Fe-Pc, in which systems no Fano line shape mode is observed. This demonstrates that electron-phonon coupling strongly depends on the property of the central metal atom. This is further confirm by photoemission spectroscopy measurements demonstrating that the alteration of the valence band upon adsorption depends of the central atom.

O 6.5 Mon 11:30 H38

Site and orbital-dependent charge donation and spin manipulation in electron doped metal-phthalocyanines — •Cornelius Krull[1], Roberto Robles[2], Aitor Mugarza[1], and Pietro Gambardella[1,3] — [1]Catalan Institute of Nanotechnology (ICN), Barcelona, Spain — [2]Centre d'Investigacions en Nanociència i Nanotecnologia (CIN2), Barcelona, Spain — [3]Institució Catalana de Recerca i Estudis Avançats (ICREA) Universitat Autonoma de Barcelona, Barcelona, Spain

Similar to silicon-based electronics, chemical doping offers a tool for tailoring the electrical characteristics of organic molecular compounds. Contrary to inorganic semiconductors, however, controlling the position of dopants and charge donation in molecular complexes is a complicated task due to the existence of multiple doping sites, electron acceptor levels, and intramolecular correlation effects. Here we use scanning tunneling microscopy to observe the position of single Li dopants within Cu-phthalocyanine and Ni-phthalocyanine molecules in contact with a metal substrate and probe the charge transfer process with unprecedented spatial resolution. We show that individual phthalocyanines can accommodate at least three stable nonequivalent doping sites and up to six dopant atoms. Ligand and metal orbitals can be selectively charged by modifying the configuration of the Li complexes. Because of strong charge-spin correlation in confined molecular orbitals, alkali atoms provide an effective way to tune the molecular spin without introducing magnetic dopants.

O 6.6 Mon 11:45 H38

Investigation of the adsorption of vanadiumoxide-phthalocyanine on Cu(111) — •Christoph Bürker[1], Alexander Gerlach[1], Jens Niederhausen[2], Steffen Duhm[3], Takuya Hosokai[4], Blanka Detlefs[5], Norbert Koch[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, DE — [2]Institut für Physik, Humboldt-Universität zu Berlin, DE — [3]Institute of Functional Nano & Soft Materials, Soochow University, CN — [4]Department of Materials Science and Technology, Iwate University, JP — [5]European Synchrotron Radiation Facility, FR

We study the adsorption geometry of the non-planar vanadiumoxide-phthalocyanine (VOPc) molecule on Cu(111) using X-ray standing wave (XSW) measurements and complementary techniques. The XSW analysis of the C 1s, N 1s, V 2p and O 1s core-levels, accompanied by simulations and scanning tunneling microscopy measurements, indicates that the molecules adsorb predominantly with their oxygen atom pointing towards the Cu(111) surface. Upon adsorption, the geometry of the VOPc molecule suffers a significant distortion compared to the molecular geometry in the crystal. Finally, we compare these results with published data of GaClPc on Cu(111) [1] and VOPc on Au(111) [2].

[1] A. Gerlach et al., *Phys. Rev. Lett.* **106**, 156102 (2011)
[2] D. A. Duncan et al., *Surf. Sci.* **604**, 47 (2010)

O 6.7 Mon 12:00 H38

Systematic X-ray standing wave study of pentacene and pentacenederivatives on coinage metals — •Alexander Gerlach[1], Christoph Bürker[1], Jens Niederhausen[2], Steffen Duhm[3], Takuya Hosokai[1], Blanka Detlefs[4], Norbert Koch[2], Georg Heimel[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, DE — [2]Institut für Physik, Humboldt-Universität zu Berlin, DE — [3]FUNSOM, Soochow University, CN — [4]European Synchrotron Radiation Facility, FR

We present X-ray standing wave data for pentacene (PEN), pentacenequinone (P2O) and pentacenetetrone (P4O) on Cu(111), Ag(111), and Au(111). The bonding distances d and the distortions of the absorbed molecules measured with this technique are characteristic for the interaction mechanism with the different substrates [1,2]. Depending on the number of C=O groups attached to the molecule we find surprisingly different bonding distances and adsorption geometries on the three coinage metal surfaces. On Au(111) [Cu(111)], there is a relatively weak [strong] interaction, i.e. $d_C \approx 3.3\,\text{Å}$ [$2.3\,\text{Å}$], with negligible [significant] distortion of the molecules. On Ag(111), as the intermediate case, both scenarios are observed: While for PEN and P2O we find a weak substrate interaction with $d_C \approx 3.0\,\text{Å}$ and $3.3\,\text{Å}$, P4O shows a chemisorptive bonding with $d_C \approx 2.7\,\text{Å}$. Finally, we discuss consequences of the different bonding behavior with regard to the electronic structure and the enery-level alignment at the organic-metal interface. [1] N. Koch et al., *J. Am. Chem. Soc.* 130 (2008) 7300 [2] A. Gerlach et al., *Phys. Rev. B* 75 (2007) 045401

O 6.8 Mon 12:15 H38

Coadsorption of Metal-phthalocyanines and PTCDA on Ag(111) — •Christoph Sauer[1,2], Marco Grünewald[3], Benjamin Stadtmüller[4,5], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie (KIT), D-76021 Karlsruhe — [3]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, D-07743 Jena — [4]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, D-52425 Jülich — [5]Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, D-52425 Jülich

By means of high-resolution photoelectron spectroscopy (PES) we demonstrate that annealing a heteromolecular film of sub-monolayers of metal-phthalocyanine (MePc) deposited on top of one monolayer (ML) of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Ag(111) results in a mixed MePc:PTCDA-monolayer. The replacement of PTCDA by the MePc is explained within a model based on intramolecular Coulomb repulsion. The PES investigation of the mixed MLs exhibits variations of the spectral signatures of the individual components with respect to the pure ML spectra on Ag(111), thus indicating significant differences in the bonding of the respective molecules. Remarkably these spectral variations are more pronounced for mixed CuPc:PTCDA-MLs than for the respective SnPc:PTCDA-ML films.

O 6.9 Mon 12:30 H38

Substrate-mediated band-dispersion of adsorbate molecular states — •Michael Wiessner[1], Peter Puschnig[2], Masashi Arita[3], Kenya Shimada[3], Achim Schöll[1], and Friedrich Reinert[1] — [1]Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg, Germany — [2]Institut für Physik, Karl-Franzens Universität Graz, Austria — [3]Hiroshima Synchrotron Radiation Center, Hiroshima University, Hiroshima 739-0046, Japan

Charge carrier mobilities in molecular condensates are usually small, since the coherent transport, which is highly effective in conventional semiconductors, is impeded by disorder and the small intermolecular coupling. A significant band dispersion can usually only be observed in exceptional cases such as for π-stacking of aromatic molecules in organic single crystals. Based on angular resolved photoemission, we demonstrate on the example of planar π-conjugated molecules, that the hybridisation with a metal substrate can substantially increase the delocalization of the molecular states in selective directions along the surface. Supported by *ab initio* calculations we show how this mechanism couples individual 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) molecules via the Ag(110) substrate within the organic layer resulting in a four times larger in-plane charge carrier mobility.

O 6.10 Mon 12:45 H38

Temperature influence on the self-assembly of phthalocyaninato complexes on gold studied by second harmonic generation (SHG). — •Nadezhda Lilichenko[1], Ulrich Glebe[2], Frank Hubenthal[1], Ulrich Siemeling[2], and Frank Träger[1] — [1]Institut für Physik, Universität Kassel and CINSaT, Germany — [2]Institut für Chemie, Universität Kassel and CINSaT, Germany

Self assembled monolayers (SAMs) attracted great attention in different fields of science. Due to their designable physical and chemical properties SAMs are used in a variety of applications, e.g. as biosensors, switchable interfaces or in molecular electronics. Phthalocyanines (Pcs) are ideal candidates for SAMs due to their outstanding optical and electronic properties.These molecules bind to the surface by multiple anchor groups and they have large footprints, which are preconditions for the formation of stable monolayers. In our experiments we have used thioether substituted (sub-)phthalocyanines for SAM formation. To extract the adsorption kinetics the film formation was monitored by optical second harmonic generation and subsequently the SHG data was fitted by the standard Lamgmuir kinetic models. Depending on the molecular structure, the adsorption can be described either by 1^{st} or 2^{nd} order Langmuir kinetic models. Additionally, the temperature and the molecular concentration of the Pc-solution has been systematically varied to optimise SAM formation. The most important result, among other, is, a strong dependence on the temperature. While for $T = 2°\text{C}$ the SAMs were only loosely packed, at $T = 25°\text{C}$ dense films are generated.

O 7: Plasmonics and Nanooptics I

Time: Monday 10:30–13:00 Location: H31

O 7.1 Mon 10:30 H31

Nanoantennas as Common Substrate for Simultaneous Surface-Enhanced Raman and Infrared Spectroscopy — •Jörg Bochterle[1], Cristiano D'Andrea[2], Frank Neubrech[1,3], Barbara Fazio[2], Pietro Gucciardi[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany — [2]CNR IPCF Istituto per i Processi Chimico-Fisici, Viale F. Stagno D'Alcontres 37, I-98156, Messina, Italy — [3]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

It is well known, that localized surface plasmon resonance (LSPR) frequency of nanoscopic metal particles, i.e. nanoantennas, is tunable by changing their geometric dimensions, such as length or widths for example. In our experiments, we utilize elongated nanoantennas with lengths of about 1 μm and widths and heights of 60 nm for the demonstration of simultaneous surface enhanced Raman scattering (SERS) and surface enhanced infrared spectroscopy (SEIRS). When exciting the nanoantennas with light that is polarized along the long axis, the nanoantennas feature LSPRs in the infrared (IR) spectral range, whereas light polarized along the short axis excites a LSPR in the visible. With molecules adsorbed on the nanoantennas, these two distinct resonances are tuned to match the optimum frequency simultaneously for SERS and for SEIRS. We present a prove of principle using methylene blue as probe molecule and achieve enhancements of the particular signals in the order of 10^3 for SERS and 10^5 for SEIRS.

O 7.2 Mon 10:45 H31

Quantitative mapping of plasmonic near-field intensity using infrared far-field vibrational spectroscopy — •Daniel Dregely[1], Frank Neubrech[1], Huigao Duan[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Key Laboratory for Micro-Nano Optoelectronic Devices of Ministry of Education, Hunan University, P.R. China

Nanoantennas confine electromagnetic fields at visible and infrared wavelengths to volumes of only a few cubic nanometers. Assessing their near-field distribution offers fundamental insight into light-matter coupling and is of special interest for applications such as radiation engineering, attomolar sensing, antenna enhanced vibrational spectroscopy [1], and nonlinear optics. Most experimental approaches to measure near-fields employ either diffraction-limited far-field methods or intricate near-field scanning techniques. Here, by diffraction-unlimited far-field spectroscopy in the infrared, we map the intensity of the electric field in the vicinity of plasmonic nanoantennas with 10 nm spatial accuracy. Specifically, we place a patch of probe molecules at different locations in the near-field of a resonant antenna and extract the molecular vibrational excitation. We map the field intensity along a dipole antenna and confirm our findings with numerical simulations. Furthermore, we quantify the near-field intensity of a gap-type antenna, observing a 5.9 times vibrational strength enhancement inside the gap.

[1] F. Neubrech et al., Phys. Rev. Lett. 101, 157403 (2008).

O 7.3 Mon 11:00 H31

Antenna enhanced sensing of surface phonon polaritons — •Frank Neubrech[1,2], Tadaaki Nagao[3], and Annemarie Pucci[1] — [1]Kirchhoff Institute for Physics, University of Heidelberg, Heidelberg, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart, Germany — [3]International Center for Materials Nanoarchitectnics, National Institute for Materials Science, Tsukuba, Japan

Excited resonantly, antenna-like nanostructures confine the electromagnetic radiation on the nanoscale and therefore enhance the electromagnetic field in their vicinity, which can be exploited for surface enhanced infrared spectroscopy. The only precondition is a good match between the fundamental resonant excitation of the nanoantenna and the vibrational signal of the adsorbate of interest. To demonstrate the influence of the vibrational signal strength on the signal enhancement we performed infrared spectroscopic measurements using Si wafers covered with SiO2 layers of different thickness. For thin layers we observe only a small change of the relative transmittance due to the SiO2 vibration. For thicker layers the coupling between the plasmonic excitation and the SiO2 surface phonon polariton becomes stronger and the relative transmission at the respective frequency increases. Layers with thickness larger than some tens of nanometers feature a transmission close to 100% at the SiO2 frequency.

O 7.4 Mon 11:15 H31

Experimental realization of an optical point-to-point connection with nanoantennas — •Daniel Dregely[1], Klas Lindfors[1,2], Markus Lippitz[1,2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany

Advances in nanofabrication in the past years allowed for the adaption of radiofrequency and microwave concepts to optical wavelengths. It was theoretically proposed that optical nano-antennas outperform direct wire connects in energy transmission on the nanoscale [1]. We experimentally realized an optical antenna link using a transmitter and a receiver antenna. We furthermore used different antenna geometries to increase the energy transmission efficiency and show that the direction of the transmitted beam can be spatially steered using phase control.

[1] A. Alù and N. Engheta, Phys. Rev. Lett. 104, 213902 (2010).

O 7.5 Mon 11:30 H31

Nonlinear optical response of complex plasmonic nanoantennas and Fano structures — •Bernd Metzger[1], Mario Hentschel[1,2], Thorsten Schumacher[1,2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

For the design of optical materials with desired functionality and optical response, we require a deep understanding of the light-matter interaction. In particular plasmonic nanoantennas have shown great potential for tailoring the linear as well as the nonlinear optical response. To gain insight into the nonlinear optical processes that occur upon illumination of these nanoantennas with strong light fields, we perform third harmonic spectroscopy of different complex nanoantenna structures using widely tunable sub-30 fs laser pulses. We find the peak efficiency of the third harmonic emission of rod-type antennas slightly red-shifted to their far-field extinction spectrum. This behavior can be understood and modeled using a classical anharmonic oscillator [1]. Furthermore, we investigate complex nanoantennas, such as dolmen-type and oligomer structures, which exhibit Fano resonances in their linear extinction spectrum. The nonlinear response of these structures is as well strongly related to their linear optical properties and originates mostly from the interplay of bright and dark modes as well as the intense localized near-fields within the metallic nanostructures.

[1] M. Hentschel et al., Nano Lett. 12, 3778 (2012).

O 7.6 Mon 11:45 H31

Tunable Nano-Cavities as optical antennas for near-field scanning probes — •Heiko Gross, Michail Kromm, and Bert Hecht — Experimental Physics 5, University of Würzburg, Germany

Plasmon resonances of nanoslit cavities at the edge of single crystalline gold flakes are experimentally characterized. Controlling the length of the slits created by focused ion beam milling enables us to tune the plasmon resonance through the visible wavelength range while still maintaining highly confined fields within the gap. Unidirectional emission is also observed from the open end of the cavity.

Exploiting the mechanical rigidness of gold flakes makes it possible to use these cavities as a scanning probe with an optical antenna to enhance the emission of single molecules at spatial resolutions well beyond the diffraction limit.

O 7.7 Mon 12:00 H31

Evolutionary optimization, realization and analysis of high-performance optical antennas — •Thorsten Feichtner[1], Oleg Selig[2], Markus Kiunke[1], and Bert Hecht[1] — [1]Nano-Optics & Biophotonics Group, Experimentelle Physik 5, Physikalisches Institut, Wilhelm- Conrad-Röntgen-Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]FOM Institute AMOLF, Biomolecular Photonics Group, Science Park 104, 1098 XG Amsterdam, The Netherlands

Optical antennas have a wide range of useful applications, e.g. increase of solar cell absorption, coupling of energy into plasmonic waveguides or enhancement of single emitter decay rates. Most nano antenna designs so far are based upon radio wave antenna technology which might not yield optimal performance. Structures with enhanced optical properties can be found by means of evolutionary algorithms [1]. We present an extension of this concept to geometries suitable for nano-fabrication, where we use structures with rounded edges and feature sizes of 22 nm that are described by a binary square matrix containing '0' and '1'. We show in experiments using two-photon-photoluminescence that the resulting evolutionary nano-antennas indeed show a two-fold increase compared to linear dipolar two-wire nano-antennas as suggested by simulations. We also outline a theory explaining this surprising finding based on the reciprocity theorem.

[1] Feichtner, T., Selig, O., Kiunke, M. & Hecht, B. Evolutionary Optimization of Optical Antennas. Physical Review Letters 109, 127701 (2012).

O 7.8 Mon 12:15 H31

Using low-loss phase-change materials for IR antenna resonance tuning — •Ann-Katrin U. Michel, Tobias W. W. Mass, and Thomas Taubner — 1st Institute of Physics, RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany

Metallic nanoantennas are able to produce significantly enhanced and highly confined electromagnetic fields. The variation of nanorod material, geometry and substrate allows a wide tuning range of their resonance frequency.

We show a concept for resonance tuning of aluminum nanorods with defined geometry via variation of the refractive index n of an embedding medium. Phase-change materials (PCM) offer a huge contrast in n due to a phase transition from amorphous to crystalline state, which can be thermally triggered. Due to a negligible small imaginary part of the dielectric function of both phases, in the mid-IR resonance damping is avoided. Exemplary we used the two PCM InSb and $Ge_3Sb_2Te_6$ [1],which provide a huge contrast in n and a negligible small losses in the mid-IR spectral range. We present resonance tuning to lower as well as to higher wavenumbers with a maximum shift of about 11.5%, which is confirmed via FDTD simulations.

Since nanoantennas represent a model system for metamaterials, our study enable a variety of new applications for sensing, enhanced IR spectroscopy [2] and programmable optical nanostructures [3].

[1] Sittner et al. *Phys. Status Solidi A* **2012**.

[2] Adato et al. *PNAS* **2009** 106(46), 19227-19232.

[3] Xingjie Ni et al. *Science* **2012** *335*, 427.

O 7.9 Mon 12:30 H31

Extreme ultraviolet light generation enhanced by plasmonic nanostructures — •Murat Sivis[1], Matthias Duwe[1], Bernd Abel[2], and Claus Ropers[1] — [1]Materials Physics Institute and Courant Research Centre, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Leibniz Institute of Surface Modification, University of Leipzig, Permoserstr. 15, 04318 Leipzig

The near-field enhancement in metallic nanostructures can be used to study numerous strong-field effects within confined volumes, such as the generation of extreme ultraviolet (EUV) light. [1,2] Here, we present a comprehensive study of highly nonlinear processes in plasmonic nanostructures, including resonant bow-tie antennas as well as tapered hollow waveguides. In particular, we will discuss the excitation mechanisms and spectral characteristics of nanostructure-enhanced fluorescent line emission from noble gases. To this end, we have developed a method to gauge plasmonic fields in nanostructures, which is based on the spectral fingerprint of strong-field fluorescence. Prospects and limitations of EUV generation in nanoscopic volumes will be elucidated.

[1] S. Kim, *et al.*, Nature **453**, 757 (2008)
[2] M. Sivis, *et al.*, Nature **485**, E1 (2012)

O 7.10 Mon 12:45 H31

Nanoantenna supported internal photoemission in metal-isolator-metal junctions — Dieter Akemeier[1], Detlef Diesing[2], Dominik Differt[1], Adelheid Godt[3], Ingo Heesemann[3], •Matthias Hensen[1], Andreas Hütten[1], Walter Pfeiffer[1], and Christian Strüber[1] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Fakultät für Chemie, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany — [3]Fakultät für Chemie, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

Thin-film metal-isolator-metal (MIM) heterosystems, i.e. Ta-TaO$_x$-Ag and Ta-TaO$_x$-Au junctions, are investigated as devices for ultrafast nanoscale electron injection in nanophotonic applications. Internal photoemission (IPE) microscopy provides lateral maps of the induced multiphoton photocurrents that are excited by few-cycle pulses from a Ti:Sapphire laser (6 fs). Nanostructures acting as optical antennas are prepared on the Ag top electrode by deposition of Au nanoparticles and Au nanoparticle aggregates or by means of local focussed ion beam milling. The multiphoton internal photoemission current is strongly enhanced in the vicinity of these nanoantennas. Based on FDTD model calculations (a grid-based differential time-domain numerical modeling method) this enhancement is attributed to field enhancement effects in the MIM structure.

O 8: Surface Chemical Reactions and Heterogeneous Catalysis I

Time: Monday 10:30–13:15 Location: H33

O 8.1 Mon 10:30 H33

Influence of the nanometer scale on the reactivity of cerium dioxide — •Kostiantyn Kulyk and Mykola Borysenko — Chuiko Institute of Surface Chemistry, National Academy of Sciences of Ukraine, General Naumov Str. 17, 03164 Kyiv, Ukraine

Cerium dioxide is considered as the most widely used rare-earth oxide in industry due to its unique redox properties and elevated oxygen storage capacity. However, the preparation of ceria nanoparticles with desired size still remains a challenge and to date little is known about how the nanometer scale of the ceria particles effect its chemical behavior. My talk will illustrate the crucial points of our novel method of synthesis of ceria nanoparticles supported on fumed silica. The proposed method allows us to synthesize nanocomposites with a controllable size of cerium dioxide crystallites from 3 to 24 nm (XRD, Solid State MAS ^{29}Si NMR, Raman, IR, SEM, UV-vis). Comparison of reactivity of nanosized CeO$_2$ and micrometer scale CeO$_2$ will be demonstrated by studying the interaction of nanocomposites with cerium acetylacetonate, acetylacetone, acetic acid, thiazolyl- and benzothiazolyl substituted coumarines. Mechanisms and kinetics (n, E$_{act}$, k$_o$, dS) of surface reactions were studied using a temperature programmed desorption mass spectrometry (TPD-MS) and TG/DTG/DTA. The main part of my speech will be devoted to the phenomena of dramatic enhancement of the reactivity of ceria nanoparticles resulting in its ability to chemisorb acetylacetone at room temperature and form grafted ceriumacetylacetonate groups. The mechanism of the nanoeffect will be presented and described in details.

O 8.2 Mon 10:45 H33

Adsorption and decomposition of acetic acid on ceria-based model catalysts — •A. Neitzel[1], Y. Lykhach[1], V. Johánek[2], N. Tsud[2], T. Skála[3], K. C. Prince[3], V. Matolín[2], and J. Libuda[1] — [1]FAU Erlangen-Nürnberg, Germany — [2]Charles University in Prague, Czech Republic — [3]Sincrotron Trieste, Italy

The adsorption and decomposition of acetic acid on stoichiometric CeO$_2$(111), partially reduced CeO$_{2-x}$, and Pt/CeO$_2$ thin films prepared on Cu(111) were investigated by synchrotron radiation and resonant photoelectron spectroscopy. Molecular acetic acid and acetate are the major species formed upon adsorption at 150 K. Decomposition of these species on CeO$_2$(111) does not alter the oxidation state of cerium cations. In contrast, decomposition of acetic acid on CeO$_{2-x}$ results in re-oxidation between 250 and 400 K, followed by reduction of ceria and C-C bond cleavage above 400 K. Intermediate decomposition products like formate, alkoxy, and alkyl species were identified on the surface. These were converted into thermally stable carbonaceous species above 600 K. On Pt/CeO$_2$, hydrogen spillover and reverse spillover were observed during annealing. Furthermore, CO, alkoxy, alkyl moieties, and elemental carbon were detected. Above 500 K, reverse oxygen spillover from ceria to Pt particles resulted in oxidative removal of carbonaceous species. It was found that C-C bond cleavage is promoted in presence of oxygen ad-atoms on Pt(111) and Pt/CeO$_2$. As a result, formation of methoxy species and hydroxyl groups on Pt was observed. On Pt/CeO$_2$, pre-exposed to oxygen, hydrogen reverse spillover was found to be suppressed.

O 8.3 Mon 11:00 H33

Dehydrogenation of dodecahydro-N-Ethylcarbazole on Pt(111) — •Christoph Gleichweit, Max Amende, Stefan Schernich, Wei Zhao, Oliver Höfert, Jörg Libuda, Hans-Peter Steinrück, and Christian Papp — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen (Germany)

The dehydrogenation of the liquid organic hydrogen carrier dodecahydro-N-ethylcarbazole (H$_{12}$-NEC) on Pt(111) was studied by high-resolution X-ray photoelectron spectroscopy (HR-XPS) in order to elucidate its dehydrogenation mechanism. H$_{12}$-NEC was adsorbed under ultra hight vacuum (UHV) conditions by physical vapor deposition, and subsequently the reaction was monitored during heating. Although the molecules are quite complex, we identified the reaction steps after detailed analysis of the C1s and N1s core levels. During adsorption at low temperatures the development of monolayer and multilayer peaks was observed. Interestingly the N1s peak assigned to the multilayer is found at lower binding energy than the monolayer peak. When heating the sample continuously, the multilayer desorbs up to temperatures of about 285 K while the signature of the monolayer increases due to decreased damping. Subsequently, the dehydrogenation of the H$_{12}$-NEC to NEC follows successively in the range of 280 K to 500 K. Above 430 K the dealkylation reaction of the NEC to carbazole is observed. Upon further heating to 1000 K decomposition to adsorbed carbon takes place. We acknowledge the cluster of excellence “Engineering of Advanced Materials”.

O 8.4 Mon 11:15 H33

O K-edge NEXAFS for Silica-Supported Molybdena at Different Loadings: theoretical cluster studies — •Lili Sun[1], Klaus Hermann[1], Kazuhiko Amakawa[1], Michael Hävecker[2], Anette Trunschke[1], and Robert Schlögl[1] — [1]Inorganic Chemistry Department, Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin (Germany). — [2]Department of Solar Energy Research, Helmholtz-Zentrum Berlin/BESSY II, Albert-Einstein-Str. 15, 12489 Berlin. Germany.

Oxygen core excitations in different molybdena-silica clusters are evaluated using density-functional theory to explain the X-ray absorption fine structure (NEXAFS) near the O K-edge measured for molybdena supported by SBA-15 silica. Different oxygen species in the molybdena-silica clusters with molybdenum in different coordination can be clearly distinguished in the theoretical spectrum. The experimental NEXAFS spectra at low molybdenum loadings ($< 6.6\%$) exhibit a double-peak structure in the O 1s to Mo 4d / O 2p excitation range of 529-536eV. This is reproduced by the theoretical results for tetrahedral dioxo MoO_4 units, singly or doubly connected with the silica substrate. The experimental spectrum shows a transition from a double- to a broad asymmetric single-peak structure at high molybdenum loadings (about 13.3%). This can be modeled by decreasing the distance between the two molybdenyl oxygen atoms in the dioxo MoO_4 unit leading to direct O-O coupling. Thus, the spectral transition may be explained by a simple structural effect resulting from the increased density (squeezing) of MoO_4 units at the SBA-15 silica surface.

O 8.5 Mon 11:30 H33

DFT study of Redox-Active Metal-Organic Frameworks — •Jelena Jelic[1], Dmytro Denysenko[2], Dirk Volkmer[2], and Karsten Reuter[1] — [1]TU Munich, Germany — [2]University of Augsburg, Germany

Next to applications in gas storage or drug delivery, metal-organic frameworks (MOFs) also receive increasing attention as redox active catalysts. We have recently reported on a Co-based MOF within the robust and modular MFU-4 structural family that shows promising reversible gas-phase oxidation properties [1]. We here present a density-functional theory (DFT) based computational screening approach to identify other coordinatively unsaturated metal centers or ligands that yield even more redox-active frameworks. A central concern is the accuracy of present-day DFT functionals, and we elucidate systematic shortcomings of semi-local DFT in order to establish it as a reliable and computationally efficient tool for extended in-silico searches. Among the tested ligands hydrides seem particularly promising and we further scrutinize this by detailed mechanistic analysis of potential oxidation reactions.

[1] D. Denysenko, T. Werner, M. Grzywa, A. Puls, V. Hagen, G. Eickerling, J. Jelic, K. Reuter, and D. Volkmer, Chem. Commun., 1236 (2012)

O 8.6 Mon 11:45 H33

Identifying Cu(I) Cationic Positions in SSZ-13 by Modeling Infrared and Diffuse Reflectance Spectra — •Florian Göltl[1], Philippe Sautet[1], Kerstin Hummer[2], Georg Kresse[2], and Jürgen Hafner[2] — [1]University of Lyon I, ENS Lyon, Allee d'Italie 46, 69342 Lyon, France — [2]University of Vienna, Faculty of Physics, Computational Materials Physics, Sensengasse 8/12, 1090 Vienna, Austria

Copper containing zeolites are prime candidates in removing nitrous oxides from exhaust gases. Recently an especially high activity of Cu containing SSZ-13 for the given reaction has been shown in experiment. However, the exact cationic positions within this material have been debated. Based upon the catalyst preparation process we suggest a new type of Cu(I) site within SSZ-13. We use density functional to model different active sites and the IR spectrum of adsorbed CO. We find two different peaks, one redshifted by 2-5 cm^{-1}, the other one red-shifted by 15 cm^{-1}. Furthermore we calculate the optical absorption spectra of those sites using Bethe-Salpeter Equation on top of self consistent GW_0 calculations. Compared to hybrid functoinal calculations the GW_0 approximation increases the energy gap between Cu 3d- and 4s states by about 2 eV. On the other hand, excitonic effects calculated within Bethe-Salpeter Equation reduce this gap upon optical absoption by about 3 eV, which leads to absorption maxima for the Cu d-s transition of 4 eV and between 4.5 and 4.7 eV for different cationic sites. Our calculations agree perfectly with experiment.

O 8.7 Mon 12:00 H33

Interfacial complexation reaction in vacuo by metal-organic chemical vapour deposition — •Anthoula C. Papageorgiou[1], Sybille Fischer[1], Seung Cheol Oh[1], Francesco Allegretti[1], Alissa Wiengarten[1], Knud Seufert[1], Saranyan Vijayaraghavan[1], Katharina Diller[1], Robert G. Acres[2], Kevin C. Prince[2], Florian Klappenberger[1], Willi Auwärter[1], Joachim Reichert[1], and Johannes V. Barth[1] — [1]Physik Department E20, Technische Universität München, 85748 Garching, Germany — [2]Sincrotrone Trieste, 34149 Basovizza, Italy

The fabrication and control of metal coordination compounds or architectures at well-defined interfaces is a thriving research domain with promise for various areas, including single-site catalysis, molecular magnetism, light-harvesting and molecular rotors and machines. To date such systems have been realized either by grafting prefabricated metal-organic complexes or by protocols combining molecular linkers and single metal atoms at the interface. Here we report a different pathway employing metal-organic chemical vapour deposition, as exemplified by the reaction of meso-tetraphenylporphyrin derivatives on atomistically clean Ag(111) with a metal precursor under vacuum conditions. STM, XPS and NEXAFS reveal the formation of a meso-tetraphenylporphyrin cyclodehydrogenation product that readily undergoes metalation after exposure to the metal precursor vapour and thermal treatment. A self-terminating porphyrin metalation protocol, which proceeds without additional surface-bound by-products, yielding a single, thermally robust layer of metalloporphyrins, is discovered.

O 8.8 Mon 12:15 H33

Surface activated dedeuteration of deuterofullerenes — Seyithan Ulas, Patrick Weis, •Artur Böttcher, and Manfred Kappes — Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

Deuterofullerenes have been created by exposing C_{60} films grown on Au(111) to atomic deuterium. The composition of the films created is dominated by $C_{60}D_{18}$ and $C_{60}D_{36}$. The thermally induced decomposition of the deuterofullerenes proceeds via emission of D_2, C_{60} and $C_{60}D_{x<46}$. The $C_{60}D_x$/Au(111) interface has been found to be responsible for the D_2 emission observed. The catalytic role of the Au(111) surface resembles the activated dedeuteration of deuterofullerenes as induced by alkali metal doping /1/. A lower limit to the D_2/D conversion yield (integrated D_2 emission/D exposure) as induced by C_{60} on Au(111) has been estimated to be higher than 10^{-4}. D_2 emission competes with cage fragmentation which leads to gradual graphitization of the Au(111) surface. The latter process corresponds to poisoning of the catalyst.

/1/ D. Löffler et al. J. Phys. Chem. C, 112 (2008) 13796

O 8.9 Mon 12:30 H33

Density Analysis of 1-Octadecanethiol (CH3 (CH2)17-SH) and 1-Hexadecanethiol (CH3 (CH2)15-SH) Self-Assembled Monolayers (SAMs) on Gold and Silver by Impedance Spectroscopy — •Uddin Md. Jalal, Nivedita Yumnam, and Veit Wagner — School of Engineering and Science, Jacobs University, Campusring 1, D-28759 Bremen, Germany

Self-assembled monolayers (SAMs) have significantly contributed to the field of interfacial electron transfer, to developing electrodes, to fabricating lipid bilayers on electrodes among others. For applications high quality self-assembled monolayers (SAMs) with low leakage currents and without pinholes are important.

In this study we measured the impedance of 1-Octadecanethiol (CH3 (CH2)17-SH) and 1-Hexadecanethiol (CH3(CH2)15-SH) based SAMs on gold (Au) and silver (Ag) surfaces prepared on polyethylene terephthalate (PET) flexible substrates to assess the quality of the SAM layers. For optimization of the quality of SAM layers on Au and Ag surfaces, the adsorption time of Octadecanethiol (CH3 (CH2)17-SH) and Hexadecanethiol (CH3 (CH2)15-SH) on gold and silver was systematically varied from 30 seconds to 24 hours. Adsorption times beyond 1 hour were found to have negligible difference in layer quality. To be able to sense leakage current for those high quality layers, low noise and low frequency measurement at 1Hz were necessary. The impedance data analyzed using an R-C model reveals that the SAMs of (CH3(CH2)15-SH) have lower leakage current in comparison to the SAMs of (CH3(CH2)17-SH).

O 8.10 Mon 12:45 H33

Dissociative adsorption of water on stepped metal surfaces — •Davide Donadio[1], Rengin Pekoez[1], Svenja Woerner[1], Luca Ghiringhelli[2], and Luigi Delle Site[3] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Fritz Haber Institute, Berlin, Germany — [3]Freie Universität Berlin, Germany

Water-metal interfaces play a key role in many chemical processes, from catalysis to corrosion and photoelectrochemistry. Whereas water adlayers on atomically flat transition metal surfaces have been investigated in depth, little is known about water on stepped surfaces [1].

Using first-principles simulations we study the adsorption of water on stepped Pt, Pd, Rh, Ni and Ir surfaces. We find that the chemistry of water at steps is in general different and cannot be predicted based on the acquired knowledge on flat surfaces. For example at Pt steps, in contrast with flat surfaces, water molecules dissociate forming mixed hydroxyl/water structures, through an autocatalytic mechanism promoted by hydrogen bonding [2]. Similar effects are analyzed systematically for several metals, and general trends are devised. Together with the attitude of water chains on metal steps to transfer protons via thermally activated hopping, these findings candidate these systems as viable proton wires.

[1] A. Hodgson and S. Haq, Surf. Sci. Rep. 64, 381 (2009).

[2] D. Donadio, L. M. Ghiringhelli and L. Delle Site, J. Am. Chem. Soc. 134, 19217 (2012)

O 8.11 Mon 13:00 H33

Auto-catalytic creation of active sites?! Step formation during NO reduction at Pt(110) — •Tongyu Wang[1], Qian Liu[2], Joost W.M. Frenken[2], and Karsten Reuter[1] — [1]TU München, Germany — [2]Leiden University, The Netherlands

We report a surprisingly distinct faceting of Pt(110) into vicinal orientations with highly regular step lattices during the near-ambient NO reduction by H_2. Reactor Scanning Tunneling Microscopy (STM) measurements demonstrate that the step density can be reversibly tuned by the NO/H_2 partial pressure ratio. In view of the potential role of steps in the reaction, this could reflect a unique self-promoting feature. We analyze these observations through first-principles atomistic thermodynamics calculations. They predict the formation of a high-coverage NO phase precisely over the experimentally employed (T,p)-range. Surface stress calculations show that the highly repulsive interaction in this adlayer builds up a huge compressive stress. This stress is accommodated by the expansive, lateral relaxation that the Pt surface can perform, when either space (grooves) or 'overhang'-type geometries (steps) are created. We thus suggest surface stress relaxation as atomic-scale origin behind the observed faceting.

O 9: Nanotribology

Time: Monday 10:30–13:00 Location: H42

O 9.1 Mon 10:30 H42

The Interdependence of Timescale and Temperature on Nanoparticle Friction — •Michael Feldmann, Dirk Dietzel, and André Schirmeisen — Institut für Angewandte Physik, JLU Giessen, Germany

In the endeavor to understand friction for a broad range of contact area sizes, friction measurement employing nanoparticle manipulation has emerged as a valuable experimental technique [1]. While the friction of nanoscopic point-like contacts have already been widely examined, investigations of more extended contacts as realized by sliding nanoparticles have recently been intensified. Here we present a study of nanoparticle friction measurements conducted with an atomic force microscope (AFM) in UHV, examining the dependence of friction on temperature and velocity [2]. A strongly non-monotonic relation between friction and temperature/velocity is observed, which cannot be explained in terms of classical models of nanoscale friction. We therefore introduce a model based on the Prandtl-Tomlinson concept, including a characteristic time evolution of the contact energy barrier. The corresponding simulations are in very good agreement with the experimental findings including the non-monotonic temperature/velocity dependence.

[1] Dietzel, D., Herding, C., Feldmann, M., Phys. Rev. B 82, 35401 (2010)

[2] Feldmann, M., Dietzel, D., Schirmeisen, A., *to be published*

O 9.2 Mon 10:45 H42

Superlubric sliding of metallic nanoparticles: The influence of contact area and orientation — •D. Dietzel[1], M. Feldmann[1], H. Fuchs[2], U. D. Schwarz[3], and A. Schirmeisen[1] — [1]Institute of Applied Physics, University of Giessen — [2]Institute of Physics, University of Muenster — [3]Yale University, New Haven, USA

Superlubricity, or also termed structural lubricity, is a fundamental concept where ultra-low friction between atomically flat surfaces can originate from the lattice mismatch at the interface. But while the basic principle is intriguingly simple, unambiguous experimental identification of structural lubricity is often problematic and can best be achieved by analyzing characteristic features unique to structural lubricity. Two of the most significant features are the distinct contact area dependence of friction and the dependence on relative orientation between nanoparticle and substrate: Theory predicts a decrease of shear stress with contact area and the existence of distinct orientations of pseudo-commensurability with sharp peaks in friction. To measure the interfacial friction we have manipulated metallic nanoparticles of different size on atomically flat surfaces by contact mode atomic force microscopy techniques. Our results confirm the sublinear scaling of friction with contact area. Moreover, we could identify different scaling for amorphous and crystalline particles in good agreement with theoretical predictions. In case of the crystalline Gold particles, we could also observe abrupt friction changes due to nanoparticle rotation. By measuring the relative orientation between particle and substrate such friction changes can be related to orientations of pseudo-commensurability.

O 9.3 Mon 11:00 H42

Unraveling and eliminating dissipation mechanisms in contacts of polymer-bearing surfaces — •Sissi de Beer and Martin H. Müser — Jülich Supercomputing Centre, Institute for Advanced Simulation, FZ Jülich, Jülich, Germany

Polymer brushes are well known to lubricate high-pressure contacts, because they can sustain a high normal load while maintaining low friction at the interface. Depending on the contact-geometry, direction of motion and brush characteristics, different dissipation mechanisms dominate the friction forces. For example, in a parallel plate geometry the interdigitation of the opposing polymers determines the lubricity, while for spherical star polymers in relative motion, viscoelastic deformation governs the energy dissipation. We discuss the relative importance of the dissipation channels for real contacts and show via molecular dynamics simulations that, by using an asymmetric contact of a hydrophobic and hydrophilic polymer-bearing surface, the important dissipation-mechanisms - interdigitation and capillary break-up - can be eliminated. This can reduce friction by a few orders of magnitude compared to a symmetric contact. Our proposed system therefore holds great potential for applications in industry.

O 9.4 Mon 11:15 H42

Correlating contact area and friction of laser-textured surfaces — •Nikolay Prodanov[1,2] and Martin H. Müser[1,2] — [1]Department of Materials Science and Engineering, Saarland University, Campus 66123 Saarbrücken, Germany — [2]Jülich Supercomputing Centre, Institute for Advanced Simulation, FZ Jülich, Jülich, Germany

Laser surface texturing (LST) is a technique for producing surfaces with a sinusoidal topography. We conduct numerical contact mechanics simulations, which are based on experimentally determined height profiles, to investigate how the kinetic friction of such surfaces is related to the real contact area.

The Green's function molecular dynamics method is used in the calculations. Surface topographies of a flat steel substrate and a bearing ball are used. The periodicity of the grooves is 9 and 18 microns. Parallel and perpendicular relative orientations of the grooves are considered. To ascertain the effect of the roughness on different length scales, we use Gaussian or Fourier smoothing of the original topographies. The dependencies of the relative contact area and of the contact pressure distribution on load, relative orientation and smoothing are obtained. The contact area is very sensitive to the spatial resolution of the topographies. The ratio of the value of real contact area at the two orientations is insensitive to smoothing. The experimental differences for the kinetic friction are similar in magnitude to those for the relative contact area. The contact pressure distribution is not sensitive to changes in the normal forces and orientations of the surfaces. Changing the resolution considerably affects the distribution.

O 9.5 Mon 11:30 H42

Friction and atomic-scale wear of graphitic lubricants on SiC(0001) in dry sliding — •Felix Wählisch[1], Judith Hoth[1], Christian Held[1], Thomas Seyller[2], and Roland Bennewitz[1] — [1]INM Leibniz-Institute for New Materials and Experimental Physics, Saarland University, Campus D2 2, 66123 Saarbrücken, Germany — [2]Technische Universität Chemnitz, Institut für Physik, Technische Physik, Reichenhainer Straße 70, 09126 Chemnitz, Germany

Sliding friction experiments on graphene grown on SiC(0001) have been performed using a combination of a microtribometer with an atomic force microscope (AFM) allowing for the investigation of atomic-scale wear. The graphene layer delaminates within ten sliding cycles starting from substrate step edges. After run in, friction is dominated by the interaction between a changing configuration of asperities at the probe sphere and a graphitic interface layer terminating the SiC substrate. Friction varies unpredictably due to changes in the contact configuration. However, the linear relation between friction and contact area can be confirmed and a shear strength as low as a few MPa is found for the contact between ruby and the graphitic layer on SiC, which remains intact under continuous sliding.

O 9.6 Mon 11:45 H42

Electrochemical control of friction in an ionic liquid — •Florian Hausen[1], Judith Hoth[1], James Sweeney[2], Robert Hayes[2], Grant B. Webber[2], Frank Endres[3], Mark W. Rutland[4], Roland Bennewitz[1], and Rob Atkin[2] — [1]INM - Leibniz-Institute for New Materials, Campus D2 2, 66123 Saarbrücken, Germany — [2]Centre for Advanced Particle Processing and Transport, The University of Newcastle, Callaghan, NSW 2308, Australia — [3]Institute of Particle Technology, Clausthal University of Technology, Arnold-Sommerfeld-Strasse 6, 38678 Clausthal, Germany — [4]Department of Chemistry, Royal Institute of Technology, Drottning Kristinas Väg 51, SE-10044 Stockholm, Sweden

Ionic liquids are potential novel lubricants due to some unique properties which can be changed systematically by variation of the ion structures. Ionic liquids form ordered layers of anions and cations at solid interfaces which can be probed by atomic force microscopy and controlled by varying the electrode potential. Friction force microscopy with colloidal probes and sharp tips has been performed under electrochemical control to reveal the influence of the ordered layers of the ionic liquid [Py1,4][FAP] on the tribological behaviour of gold [1]. It is found that friction forces decrease for negative potentials which is attributed to a lubricating effect of the cation. The control of friction in ionic liquids by electrochemical potentials is based on confined ionic liquid layers rather than on a modification of the underlying surface itself as observed for aqueous electrolytes.

[1] J. Sweeney, et al., Phys. Rev. Lett. 2012, 109, 155502

O 9.7 Mon 12:00 H42

Molecular friction at electrodes — Nikolay Podgaynyy, Sabine Wezisla, Shahid Iqbal, and •Helmut Baltruschat — Inst. f. Physikal. Chemie, 53117 Bonn, Roemerstr.164

Friction under ambient conditions often involves wet surfaces, and thus electrochemical interfaces. Yet measurements of friction at an atomic scale under electrochemical conditions are scarce.[1] We will present friction measurements performed on Au(111) single crystal electrodes and the effect of adsorbates on atomic stick-slip resolution. At the small normal load of 15 nN transition to atomic stick-slip resolution is observed, when sulfate is adsorbed on the surface. The reason for that transition could be a penetration of the tip in to the double layer. At the pzc on clean gold stick-slip behaviour does not show any transition or penetration effects. The adhesion on the force-distance curve disappear with a copper adsorption. However, with a monolayer of Cu on Au(111) a transition to stick-slip behavior is present, but without atomic resolution. Multiple slip was also observed. We will further report on the influence of the molecule orientation of pyridine adsorbed to Au(111). Molecular stick slip was also observed; the corrugation correlates with the molecule separation as determined by STM. [2]. [1]*M. Nielinger, H. Baltruschat, Physical Chemistry Chemical Physics 2007, 9, 3965.; F. Hausen, M. Nielinger, S. Ernst, H. Baltruschat, Electrochimica Acta 2008, 53, 6058. [2]*W. B. Cai, L. J. Wan, H. Noda, Y. Hibino, K. Ataka, M. Osawa, Langmuir 1998, 14, 6992.

O 9.8 Mon 12:15 H42

Chemical effects on the frictional characteristics of Pt(111) and a Pt-based metallic glass — •Arnaud Caron[1], Dmitri V. Louzguine-Luzgin[2], and Roland Bennewitz[1] — [1]INM - Leibniz-Institute for New Materials, Saarbrücken, Germany — [2]WPI-Advanced Institute of Materials Research, Tohoku University, Sendai, Japan

Nanometer-scale friction measurements on a Pt(111) surface and a Pt-based metallic glass surface have been performed in ultra high vacuum and at room temperature by using oxidized silicon and diamond coated silicon AFM-tips as counter bodies. Neither the load dependence of friction nor its velocity dependence are affected by the structural difference between the Pt(111) and the Pt-based metallic glass surfaces. However, we find that the friction forces greatly depend on the chemistry of the counter body, i.e. SiO2 or diamond. For the SiO2/Pt(111) and SiO2/Pt-based MG friction couples we measure a friction coefficient COF = 0.05. In these cases the friction is determined by the adhesive contact between the involved surfaces that gives rise to intermittent sliding. For the diamond/Pt(111) and diamond/Pt-based metallic glass friction couples we measure COF = 0.002. There the relative motion between tip and sample surface did not exhibit any stick slip. The results are discussed on the basis of Pt-silicides formation and solid solution alloying between tip and sample surfaces.

O 9.9 Mon 12:30 H42

The effect of tip force field symmetry on atomic manipulation — •Matthias Emmrich, Maximilian Schneiderbauer und Franz J. Giessibl — Institute of Experimental and Applied Physics, Universität Regensburg, 93040 Regensburg, Germany

In the last years, significant progress has been made in understanding the manipulation of adatoms on atomically flat surfaces by scanning probe microscopy. Pushing, pulling and sliding atomic manipulation modes have been identified [L. Bartels et al., PRL 1997]. Moreover, the forces that act during manipulation have been measured [M. Ternes et al., Science 2008]. In the first demonstration of atomic manipulation by Eigler and Schweizer [M. Ternes et al., Science 2008], van-der-Waals forces have been identified to allow the lateral manipulation of Xe on Ni (110). Van-der-Waals forces only depend on distance, but in later experiments involving metallic adatoms, metallic bonding was expected to contribute. Recently, a strong angular dependence of these short-range bonding forces has been measured [J. Welker and F.J. Giessibl, Science 2012].

In this study we investigate the influence of the symmetry of the tip's force field on the lateral manipulation of a CO molecule over a Cu(111) surface. The symmetry of the tip is determined using the COFI (carbon oxide front atom identification) method recently introduced by Welker and Giessibl. Lateral forces are extracted from line scans over the CO molecule at different heights. These forces were evaluated not only for different tip symmetries, but also as a function of the direction of manipulation.

O 9.10 Mon 12:45 H42

Measuring the directionality of a chemical bond with lateral force microscopy — •Daniel Meuer[1], Alfred J. Weymouth[1], Pingo Mutombo[2], Martin Ondráček[2], Thorsten Wutscher[1], Pavel Jelinek[2], and Franz J. Giessibl[1] — [1]University of Regensburg, Regensburg, 93053, Germany — [2]Institute of Physics of Czech Academy of Science, Prague, CZ-162 53, Czech Republic

Lateral forces control friction [1] and diffusion processes of adsorbates on a surface [2]. Lateral forces can be extracted from 3D normal force measurements [3]. In this contribution we show a direct lateral force measurement by dynamic lateral force microscopy (LFM). In the past LFM has made great advances with smaller oscillations, presenting atomic-scale observations on Si(111)-7x7 [4] and graphite [5]. We resolve lateral bond stiffnesses in a sample that is expected to show a strong azimutal dependence of lateral stiffnesses: the hydrogenated Si(100) surface. The "rocking horse"-type Si dimers change their orientations by 90° over a single atomic step, correspondingly, the experiment shows clearly a significant difference between the two directions. Furthermore the DFT-based calculations indicate that the tip oscillation induces a significant out-of-plane motion of the Si dimer.

[1] F.J. Giessibl et al, Proc. Nat. Acad. Sci. 99, 12006 (2002).
[2] T. Sonnleitner, et al, Phys. Rev. Lett. 107, 186103 (2011).
[3] M. Ternes, et al, Science 319, 1066 (2008)
[4] S. Kawai et al, Phys. Rev. B 79, 195412 (2009).
[5] S. Kawai et al, Phys. Rev. B 81, 085420 (2010).

O 10: Nanostructures at Surfaces I

Time: Monday 10:30–13:00 Location: H45

O 10.1 Mon 10:30 H45

Realization of a single-atom transistor in silicon — •Martin Fuechsle, Jill A. Miwa, Suddhasatta Mahapatra, and Michelle Y. Simmons — Centre for Quantum Computation & Communication Technology, University of New South Wales, Sydney 2052, Australia

Scanning tunneling microscopy (STM) has been demonstrated to enable the positioning of individual atoms on metallic surfaces with unprecedented resolution [1]. However, the realization of atomic-scale logic circuits in silicon was hampered by the covalent nature of its bonds. While resist-based strategies allowed the formation of nanostructures on the silicon surface, truly atomic-scale devices, such as donor-based quantum computation devices [2], require the ability to position individual atoms within the silicon crystal with atomic precision. Here, we present a single-atom transistor based on an individual phosphorus donor patterned with a spatial accuracy of ±1 lattice site within an epitaxial silicon environment. Using STM-based hydrogen lithography, the single impurity is deterministically placed between highly-doped transport electrodes. Low-temperature measurements confirm the presence of a single donor, the charge state of which can be precisely controlled with gate voltages. We find a charging energy that is similar to the value expected for isolated P donors in bulk silicon, previously only observed by optical spectroscopy. Our work presents an important step towards scalable donor-based quantum computer architectures.

[1] D.M. Eigler and E.K. Schweizer, Nature **344**, 524 (1990); [2] B.E. Kane, Nature **393**, 133 (1998).

O 10.2 Mon 10:45 H45

First-principles investigation of monoatomic and dimer Mn adsorption on noble metal (111) surfaces — •Francisco Munoz[1,2], Aldo Romero[2], Jose Mejia-Lopez[3], and Jose Luis Moran Lopez[4] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [3]Fac. de Fisica, Pontificia Universidad Catolica de Chile, Santiago, Chile — [4]Dep. de Fisica, Fac. de Ciencias, UNAM, Mexico D. F., Mexico

A DFT-based investigation of the adsorption of Mn single atoms and dimers on the (111) surfaces of Cu, Ag, and Au is presented. The electronic structure of the Mn adatom, chemisorbed in all inequivalent surface geometries, is analyzed. For all three substrates, the most stable geometry is a Mn atom chemisorbed in a threefold coordinated site. For the dimer, the least-energy configuration corresponds to the molecule lying parallel to the surface. In this geometry, both atoms are chemisorbed in threefold coordinated sites, but with different local symmetry. It is also found that the magnetic ground-state configuration is an antiferromagnetic arrangement of the Mn atoms; however, for the Ag substrate, the ferromagnetic state is close in energy. Furthermore, the Mn_2 molecule is chemisorbed with very similar energy on various geometries. To study the dynamical motion of the dimer components, we calculated the potential energy barriers for the Mn motion at the various surfaces. We conclude that the Mn dimer moves relatively freely for Ag, in contrast to Cu and Au.

O 10.3 Mon 11:00 H45

Nanopatterning of Cu(111)/Cu2O by Focused Electron Beam Induced Processing — •Martin Drost, Fan Tu, Esther Carrasco-Burgos, Matthias Franke, Florian Vollnhals, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The fabrication of well-defined nanostructures on surfaces is an important goal in scientific research and technology. One can distinguish two general approaches: the bottom-up route, e.g., based on the self-assembly of molecules, and top-down methods like electron beam lithography to generate arbitrarily shaped structures. We target the combination of both by applying Focused Electron Beam Induced Processing (FEBIP) on a Cu(111)/Cu2O surface to fabricate nanoscaled templates for the directed self-assembly of functional molecules. The interaction with the defined controlled electron beam induces chemical changes on the oxide surface on the nanometer scale. The feasibility of this approach was investigated by a combination of Scanning Electron Microscopy (SEM), Scanning Tunneling Microscopy (STM) and Auger Electron Spectroscopy (AES). Latest results will be presented and discussed.

O 10.4 Mon 11:15 H45

Electron quantization in arbitrarily shaped Au islands on MgO thin films — •Christian Stiehler[1], Yi Pan[1], Wolf-Dieter Schneider[1], Pekka Koskinen[2], Hannu Häkkinen[2], Niklas Nilius Nilius[1,3], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Departments of Physics and Chemistry, Nanoscience Center, University of Jyväskylä, P.O. Box 35 (YFL), FI-40014 Finland — [3]Carl von Ossietzky Universität Oldenburg, Institut für Physik, D-26111 Oldenburg, Germany

Electron quantization is a fundamental phenomenon that accompanies the transition from bulk metals to nanoclusters. The associated opening of a gap at the Fermi level crucially affects various properties of the nanostructure, e.g. its electrical and optical behavior and its performance in catalytic reactions [1]. By using low-temperature STM and STS, we have investigated the electronic structure of differently shaped 2D Au islands grown on MgO/Ag(001) thin films, concentrating on the size regime of the metal-insulator transition that occurs between 50-200 atoms in gold clusters. The observed symmetries and energy positions of quantum well states were rationalized by simple analytical models as well as by a density-functional-tight-binding approach that accounts also for structural disorder in the islands. Based on a statistically relevant number of single-cluster experiments, we derived general conclusions on the size of the HOMO-LUMO gap as a function of atom count and symmetry of the metal nanostructures.

[1] M. Valden, X. Lai, D. W. Goodman, Science 281, 1647 (1998)

O 10.5 Mon 11:30 H45

Energy dependent nanoparticle deposition on a W(110) surface — Wolfgang Rosellen, •Hendrik Bettermann, Torsten Veltum, and Mathias Getzlaff — Institute of Applied Physics, University Duesseldorf

Deposited clusters and nanoparticles are rather interesting objects not only from a fundamental point of view but additionally for technological applications due to their electronic and magnetic properties which depend strongly on the particle size. The structure determination after deposition is important because it significantly influences these properties. Our contribution is focused on magnetic 3d-nanoparticles on a W(110) substrate. After creation in the gas phase by a UHV compatible Arc Ion Cluster Source (ACIS) these particles are size selected by an electrostatic quadrupole. Mass selection and acceleration are possible because 50% of the particles are positively or negatively charged. Applying a voltage to the targeted substrate allows us therefore to change the deposition energy. Our investigations are carried out by means of scanning tunneling microscopy (STM). We will report on size and structural properties of Fe/Co particles at softlanding conditions at a kinetic energy below 1 eV per atom and compare it with accelerated and decelerated particles. We demonstrate that deceleration leads to reduced deformation whereas acceleration results in leaving the softlanding regime.

O 10.6 Mon 11:45 H45

Decoration of Co island edges on Cu(111) by Fe — •Jeison A. Fischer[1,2], Soo-hyon Phark[1], Marco Corbetta[1], Dirk Sander[1], and Jürgen Kirschner[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]LFFS, Universidade Federal de Santa Catarina , Florianópolis, SC, Brazil — [3]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

We performed low temperature scanning tunneling spectroscopy (LT-STS) measurements on almost triangular bilayer Co islands on Cu(111), which were decorated along the rim by a nm wide Fe stripe. The sample was prepared by subsequent deposition of Co[1] and Fe at 300 K. We obtained energy resolved differential conductance maps for islands with different lateral size. We find that Fe decoration induces a vanishing of the well-established electronic rim state of Co [1, 2]. The Fe-decorated islands show a pronounced spatial modulation of the differential conductance within the Co core, which we ascribe to electron confinement. A quan-titative analysis [3] identifies the characteristic length of confinement. It corresponds exactly to the geometrical height of the triangular Co core, as derived from constant current topography STM images. The comparison between characteristic lengths of Fe-decorated-Co islands and pure Co islands establishes the electronic rim state as the relevant boundary for electron confinement of the latter. This leads to a smaller characteristic length for confinement in pure Co as compared to Fe-decorated islands. [1] Pietzsch et al. Phys. Rev. Lett. 96, 237203 (2006). [2] Oka et al. Science 327, 843 (2010) [3] Rodary et al. Phys. Rev. B 75, 233412 (2007)

O 10.7 Mon 12:00 H45

Dynamics of Adsorbed EBID Precursors (W(CO)6 and Co2(CO)8) and their Fragments — •Muthukumar Kaliappan[1,2], Harald Jeschke[1], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Max-von-Laue-Straße 1, 60438, Frankfurt am Main, Germany — [2]muthukumar.kaliappan@gmail.com

We investigate the fundamentals of the growth process of nano composites in electron beam induced deposition (EBID) process using first principles molecular dynamics simulation. We compare the behavior of two carbonyl precursors ($W(CO)_6$ and $Co_2(CO)_8$) on two different SiO_2 surfaces (fully hydroxylated (FOH) and partially hydroxylated (POH)) that represent realistic EBID conditions. These precursors are commonly used to obtain tungsten and cobalt composites and our 20 ps simulations illustrates that these precursors are stable and mobile on the FOH surfaces behaving similar to the gas phase molecules. However, they fragment on POH surfaces upon their interaction with the surface active sites and tend to remain localized on their bonding sites. Apart from changes in the orientation, they show no tendency for the reformation of the parent precursor molecule. Vibrations of these adsorbed species are studied by computing their power spectrum from the trajectory that provides crucial information on the nature of adsorbed precursor fragments.

O 10.8 Mon 12:15 H45

Field equation for pattern formation on ion-beam eroded surfaces including redepositional effects — •Marc Osthues, Christian Diddens, and Stefan Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

In the last decades various self-assembled spatially ordered nanopatterns on semiconductor surfaces generated by low-energy ion-beam erosion have been found in experiments. We have studied a modified damped Kuramoto-Sivashinsky equation as one representative continuum model for the formation of these surface patterns. Previous works [1,2] on modeling the redeposition mechanism taking place during the erosion process suggested that it is appropriate to take a linear and quadratic damping term into account. Using numerical simulations and approximate analytical calculations, we show that the resulting field equation for the evolution of the surface morphology for normal ion incidence exhibits a variety of patterns, such as hexagonal dot and hole structures as well as ripple structures as a function of the parameters of the system.

[1] C. Diddens, S. J. Linz, unpublished
[2] N. Anspach, S. J. Linz, J. Stat. Mech., P06023 (2010)

O 10.9 Mon 12:30 H45

Continuum modeling of particle redeposition during ion-beam erosion — •Christian Diddens and Stefan J. Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

We have thoroughly investigated the effect of particle redeposition during ion-beam erosion for normal ion incidence within the framework a continuum model. The complicated highly non-local redeposition effect can be approximated in terms of the relative surface height with coefficients depending on the surface aspect ratio. For reasonable surface morphologies, our results are universal, i.e. do not qualitatively depend on the specific details of the sputter yield, preferred erosion directions or whether one or two lateral dimensions are considered. Furthermore, we show that an interplay of erosion, diffusion and redeposition is generically able to reproduce the hexagonally arranged nanodot patterns found in experiments with semiconductor targets.

O 10.10 Mon 12:45 H45

Supported Silver Nanoparticles for Catalytic Reactions: A RHEED Study — •Stephan Bartling, Ingo Barke, Hannes Hartmann, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

Size-selected Ag clusters deposited on amorphous alumina films can act as selective and efficient nanocatalysts for the partial oxidation of propylene [1]. In this contribution we present results for *in situ* reflection high energy electron diffraction (RHEED) from soft-landed Ag clusters in the size range of a few nm. The focus is placed on the alignment between particles and substrate that is driven by cluster-surface interaction. Whereas on highly ordered surfaces pronounced alignment was particularly found for small clusters [2], on thin Al_2O_3 layers deviations from a random orientation can only be observed for large Ag clusters ($\leq$10 nm). The analysis of such spontaneous orientation along high-symmetry crystal directions parallel to the surface is assisted by *ex situ* AFM measurements.
[1] L.M. Molina et al., Catalysis Today **160**, 116 (2011)
[2] A. Kleibert et al., Phys. Status Solidi B **247**, 1048 (2010)

O 11: Graphene: Spin-orbit interaction (jointly with DS, HL, MA, and TT)

Time: Monday 11:30–13:45 Location: H17

O 11.1 Mon 11:30 H17

Impurity-induced spin relaxation time in graphene from first principles — •Dmitry Fedorov[1], Martin Gradhand[2], Sergey Ostanin[1], Igor Maznichenko[3], Arthur Ernst[1], Jaroslav Fabian[4], and Ingrid Mertig[3,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom — [3]Martin-Luther-Universität Halle, Institut für Physik, 06099 Halle, Germany — [4]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

The spin relaxation time of conduction electrons in graphene caused by carbon and silicon impurities is studied by means of our *ab initio* approach, which was recently developed for bulk systems [1] and adapted now for the film geometry. It is found that both the momentum and spin relaxation times are extremely sensitive to the position of the impurities. We show that adatoms provide spin-flip rates 4 to 5 orders of magnitude larger than in-plane impurities. Our results strongly support the adatom-induced extrinsic mechanism of the experimentally observed spin relaxation in graphene [2].

[1] M. Gradhand et al., PRB 81, 020403(R) (2010)
[2] N. Tombros et al., Nature 448, 571 (2007)

O 11.2 Mon 11:45 H17

D'yakonov-Perel' spin dephasing in single and bilayer graphene and the role of contact resistance on the spin dephasing time — Frank Volmer[1,2], Marc Drögeler[1,2], Eva Maynicke[1,2], •Nils von den Driesch[1,2], Tsung-Yeh Yang[1,2], Gernot Güntherodt[1,2], and Bernd Beschoten[1,2] — [1]II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]JARA: Fundamentals of Future Information Technology, 52074 Aachen, Germany

We investigate spin transport in both single and bilayer graphene nonlocal spin-valve devices. Similar to our previous studies on bilayer graphene [1], we observe an inverse dependence of the spin dephasing time on the carrier mobility in our single layer devices indicating the importance of D'yakonov-Perel' like spin dephasing in exfoliated single and bilayer samples.

This general trend is only observed in devices with large contact resistances (>1 kΩ). In contrast, the spin dephasing time is significantly reduced in samples with low ohmic contacts for both single and bilayer graphene indicating that an additional spin dephasing occurs underneath the spin injection and detection electrodes.

This work has been supported by DFG through FOR 912.

[1] T.-Y. Yang *et al.* Phys. Rev. Lett. **107**, 047206 (2011)

O 11.3 Mon 12:00 H17

Intrinsic and substrate induced spin-orbit interaction in chirally stacked trilayer graphene — •Andor Kormanyos and

Guido Burkard — University of Konstanz

We present a combined group-theoretical and tight-binding approach to calculate the intrinsic spin-orbit coupling (SOC) in ABC stacked trilayer graphene. We find that compared to monolayer graphene, a larger set of d orbitals (in particular the d_{z^2} orbital) needs to be taken into account. We also consider the intrinsic SOC in bilayer graphene, because the comparison between our tight-binding bilayer results and the density functional computations allows us to estimate the values of the trilayer SOC parameters as well. We also discuss the situation when a substrate or adatoms induce strong SOC in only one of the layers of bilayer or ABC trilayer graphene. Both for the case of intrinsic and externally induced SOC we derive effective Hamiltonians which describe the low-energy spin-orbit physics. We find that at the K point of the Brillouin zone the effect of Bychkov-Rashba type SOC is suppressed in bilayer and ABC trilayer graphene compared to monolayer graphene.

The the combination of group-theoretical and tight-binding approaches can be used to study the spin-orbit interaction in other quasi-two dimensional materials, such as MoS_2, as well.

O 11.4 Mon 12:15 H17

Long Electron Spin Lifetimes in Armchair Graphene Nanoribbons — •Matthias Droth and Guido Burkard — University of Konstanz, 78457 Konstanz

Armchair graphene nanoribbons (aGNR) are promising as a host material for electron spin qubits because of their potential for scalability and long coherence times [1]. The spin lifetime T_1 is limited by spin relaxation, where the Zeeman energy is absorbed by lattice vibrations [2], mediated by spin-orbit and electron-phonon coupling. We have calculated T_1 by treating all couplings analytically and find that T_1 can be in the range of seconds for several reasons: (i) Van Vleck cancellation; (ii) weak spin-orbit coupling; (iii) low phonon density; (iv) vanishing coupling to out-of-plane modes due to the electronic structure of the aGNR. Owing to the vanishing nuclear spin of ^{12}C , T_1 is a good measure for overall coherence. These results and recent advances in the controlled production of graphene nanoribbons [3] make this system interesting for classical and quantum spintronics applications.

[1] B. Trauzettel *et al.*, Nature Phys. **3**, 192-196 (2007).
[2] M. Droth and G. Burkard, Phys. Rev. B **84**, 155404 (2011).
[3] X. Zhang *et al.*, arXiv:1205.3516 (2012).

O 11.5 Mon 12:30 H17

Tunneling-induced Spin Anisotropy Barrier in Quantum Dot Spin-Valves — •Michael Hell[1,2], Maciej Misiorny[1,2], and Maarten Wegewijs[1,2,3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich — [2]JARA - Fundamentals of Future Information Technology — [3]Institut für die Theorie der Statistischen Physik, RWTH Aachen, 52056 Aachen

Spintronics employs the two fundamental properties of a each electron: its charge and its spin-dipole moment. However, recent studies indicate that the interplay of these two degrees of freedom does not exhaust the potential of spintronics when approaching the nano-scale: spin correlations between electrons, partly characterized by the spin-anisotropy, provide an independent resource of spin information, which is stored even in a simple ferromagnet and couples to the spin-dipole moment in quantum dots. The interest in spin anisotropy also emerges from the research on single-molecule magnets (SMMs) and magnetic adatoms, in which the transport is controlled by a large spin anisotropy barrier intrinsically generated by strong spin-orbit coupling. In this talk we show that such a spin-anisotropy barrier can be externally induced by the transport of spin-correlations from ferromagnets into a a spin-isotropic interacting quantum dot with large spin S>1/2 and negligible spin-orbit interaction. This proximity-induced spin-anisotropy has the hallmarks of a spintronic exchange-field of a quadrupolar nature, a generalization of the well-established dipolar exchange field. The barrier increases with the tunnel coupling, achieving values comparable to that of SMMs, but with the flexibility of electric and magnetic tuneability.

O 11.6 Mon 12:45 H17

First-principles study of the spin-orbit interaction in graphene induced by hydrogen adatoms — •Martin Gmitra, Denis Kochan, and Jaroslav Fabian — University of Regensburg

We have performed first principles calculations of the spin-orbit coupling effects in hydrogenated graphene structures, for varying hydrogen coverage densities, using the linearized augmented plane wave method as implemented in the FLEUR code. The covalent bonding between the hydrogen and carbon atoms leads to a local structural puckering of graphene sheets, giving rise to an overlap between the Dirac and sigma electrons and a giant enhancement (from roughly 0.01 to 1 meV) of the local spin-orbit interaction. The calculated effects on the band structure and the emerging spin patterns of the electronic states can be well explained by effective Hamiltonian models derived from group theoretical principles.

This work is supported by the DFG SPP 1285, SFB 689, and GRK 1570.

O 11.7 Mon 13:00 H17

Theory of the hydrogen adatoms induced spin-orbit coupling in graphene — •Denis Kochan, Martin Gmitra, and Jaroslav Fabian — University Regensburg

We have analyzed the first-principles data of the electronic structure of hydrogenation in graphene by means of group theory derived effective Hamiltonians. We propose effective models for semihydrogenated graphene as well as for graphene with a single hydrogen adatom. The chemisorption of hydrogen modifies the structural symmetry of the plane graphene in two essential ways—it breaks the pseudospin (sublattice) symmetry and induces rippling. We show that in addition to the Rashba spin-orbit interaction there emerges another spin-orbit field which is induced by the pseudospin inversion asymmetry due to the adatoms. Our realistic effective Hamiltonians should be useful for spin transport and spin relaxation investigations.

This work is supported by DFG SFB689

O 11.8 Mon 13:15 H17

Optical properties of hydrogenated graphene from first principles — •Sebastian Putz, Martin Gmitra, and Jaroslav Fabian — Universität Regensburg, Universitätsstraße 31, 93053 Regensburg

We investigate the effect of hydrogen coverage on the optical properties of single-side hydrogenated graphene from first principles. To account for different degrees of uniform hydrogen coverage we calculate the complex dielectric function for graphene supercells of various size, each containing a single additional H atom. We use the Linearized Augmented Planewave (LAPW) method, as implemented in WIEN2k, to show that the hydrogen coverage strongly influences the complex dielectric function and thus the optical properties of hydrogenated graphene. The absorption coefficient in the visible range, for example, has different characteristic features depending on the hydrogen coverage. This opens up new possibilities of determining the hydrogen coverage of hydrogenated graphene samples in the experiment by contact-free optical absorption measurements.

This work is supported by the DFG GRK 1570.

O 11.9 Mon 13:30 H17

Electron scattering and spin polarization at the graphene/Ni(111) interface — Aran Garcia-Lekue[1], Timofey Balashov[2], Marc Ollé[2], Gustavo Ceballos[2], Andrés Arnau[1,3], Pietro Gambardella[2], Daniel Sánchez-Portal[1,3], and •Aitor Mugarza[2] — [1]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 San Sebastian, Spain — [2]Catalan Institute of Nanotecnology (ICN), UAB Campus, E-08193 Bellaterra, Spain — [3]Centro de Fisica de Materiales CFM - MPC, Centro Mixto CSIC-UPV, Apdo. 1072, San Sebastian, Spain

The interaction of graphene with a metal often perturbs the unique electronic properties of Dirac electrons in graphene. This interaction can be positively exploited to engineer the Dirac bands and obtained graphene interfaces with different functionalities. In this work we study the electronic properties of graphene nanoislands grown on Ni(111) [1] by combining scanning tunnelling microscopy and ab-initio calculations. We show that the interaction with the Ni surface opens a gap and spin-polarizes the Dirac bands, which results in a spin filtering effect in the transport across the interface [2]. On the other hand, the standing wave pattern created around the nanoislands reveal an asymmetric potential that depends both on the spin and edge type, suggesting a lateral 2D spin-filter effect similar to that occurring across the interface.

[1] M. Olle et al. Nano Lett. 12, 4431 (2012). [2] V. M. Karpan et al. Phys. Rev. Lett. 99, 176602 (2007).

O 12: Invited Talk (Swetlana Schauermann)

Time: Monday 15:00–15:45 Location: H36

Invited Talk O 12.1 Mon 15:00 H36
Interaction of Gas Phase Molecules with Nanostructured Model Supported Catalysts: Thermodynamics and Kinetics — •Swetlana Schauermann — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Atomistic-level understanding of surface processes is a key prerequisite for rational design of new catalytic and functional materials. In our studies, we investigate kinetics and thermodynamics of heterogeneously catalyzed reactions and adsorption processes on nanostructured model supported catalysts to provide fundamental insights into the surface chemistry. By employing pulsed mutli-molecular beam techniques, IRAS and synchrotron-based spectroscopies on Pd/Fe3O4/Pt(111) model surfaces, we investigate the mechanistic details of complex multi-pathway surface reactions, such as hydrocarbon transformation in presence of hydrogen or selective hydrogenation of multi-unsaturated hydrocarbons, to obtain the correlations between the reactivity, selectivity and the particular structure of the catalytic surface. Complementary, single crystal adsorption calorimetry is employed to address thermodynamics of adsorption processes and surface reactions, such as e.g. adsorption and reaction of oxygen and CO. Specifically, we focus on the particle size dependence of adsorption and reaction energies to obtain a fundamental-level understanding of how the nanometer scale confinement of matter effects the energetics of surface reactions.

O 13: Focus Session: Crystalline n-type semiconducting oxides - SnO_2, Ga_2O_3, and In_2O_3 for novel devices (jointly with HL)

Traditionally, wide band gap semiconducting oxides have been synthesized as thin polycrystalline films for mainly passive components such as transparent conducting electrodes or gas sensors. More recently, however, it has been recognized that — highly pure and single-crystalline — these oxides can become semiconductor materials for active devices. Development of high quality oxides allows to study their intrinsic physics and enables potential applications in transparent (opto)electronics, power electronics, photonics, and chemical and biological sensors. This session sets a focus on crystalline SnO_2, Ga_2O_3, and In_2O_3 as n-type semiconducting oxides and gives a state-of-the-art survey of their physics including the prospects of applications. (Organizers: Oliver Bierwagen, PDI Berlin, and Saskia Fischer, HU Berlin)

Time: Monday 15:00–19:20 Location: H2

Topical Talk O 13.1 Mon 15:00 H2
Optical absorption and radiation damage in transparent conducting oxides — •Andre Schleife[1], Friedhelm Bechstedt[2], Alfredo Correa[1], and Yosuke Kanai[3] — [1]Lawrence Livermore National Laboratory — [2]Friedrich-Schiller-University Jena — [3]University of North Carolina at Chapel Hill

Transparent conducting oxides are promising semiconductors with important technological applications in various areas of optoelectronics and photovoltaics. An accurate description of *electronic excitations and their dynamics* is crucial for predictive materials design: Outer-space applications, for instance, not only require fundamental understanding of optical absorption but also of radiation damage.

This talk outlines how parameter-free computational electronic-structure techniques based on many-body perturbation theory accomplish the scientific challenge of describing the quantum-mechanical many-body nature of the electron-electron interaction. Insight will be provided into quasiparticle and excitonic effects affecting optical properties of magnesium-, cadmium, and tin-oxide compounds. The impact of free electrons on the optical band gap will be discussed as an important real-structure effect, e.g. in *n*-doped cadmium oxide.

In addition, this talk will outline high-performance first-principles computational schemes for accurately characterizing non-adiabatic dynamics of electrons and nuclei: Understanding the *electronic stopping* and defects, e.g. when fast hydrogen atoms penetrate magnesium oxide, is essential for developing materials with high radiation resistance. Partly prepared by LLNL under Contract DE-AC52-07NA27344.

O 13.2 Mon 15:30 H2
Anisotropic dielectric function and carrier density of rutile SnO_2 — •Christian Lidig[1], Karsten Lange[1], Martin Feneberg[1], Maciej Neumann[2], Norbert Esser[2], Mark E. White[3], Min-Ying Tsai[3], Oliver Bierwagen[3,4], James S. Speck[3], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung für Materialphysik — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V. , Berlin — [3]University of California, Santa Barbara, USA — [4]Paul-Drude-Institut, Berlin

The anisotropic dielectric function of rutile SnO_2 is presented from 0.04 eV up to 20 eV. The results were obtained on a sample grown on TiO_2 having the optical axis in plane. After modelling the layer stack and taking surface roughness into account, the full dielectric function is extracted wich is compared with theoretical calculations. It turns out that electron-hole interaction influences the dielectric function up to 20 eV resulting in a pronounced redshift and redistribution of oscillator strength of features related to van Hove singularities.
Additionally, infrared spectroscopic ellipsometry was performed on a series of SnO_2:Sb layers grown on r-plane sapphire. The plasmon-longitudinal optical phonon- coupling modes yield results for the free carrier concentrations which are discussed in detail.

Topical Talk O 13.3 Mon 15:45 H2
Growth from the melt of high-quality In2O3 and Ga2O3 single crystals — •Roberto Fornari, Zbigniew Galazka, Reinhard Uecker, and Klaus Irmscher — Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin

Because of their interesting properties semiconducting oxides, in particular Ga2O3 and In2O3, have recently received much attention. However, as they were deposited as films on hetero-substrates their quality was quite poor. The growth of high-quality bulk Ga2O3 and In2O3 and manufacture of the corresponding substrates can allow the deposition of high-quality epilayers with lower residual carrier density and fewer extended defects. For this reason IKZ has undertaken an effort to grow large single crystals of these oxide compounds from the melt. Transparent semiconducting Ga2O3 single crystals with diameter of about 20 mm and 50-60 mm long were grown by the Czochralski method along the b-axis, using an Iridium crucible and a dynamic protective atmosphere to minimize the dissociation of Ga2O3 melt and ingot. In the case of In2O3 the Czochralski technique is not applicable and it was necessary to develop a novel melt growth method. This new method indeed supplied crystals from which oriented substrates could be prepared. In this presentation the melt growth of Ga2O3 and In2O3 single crystals will be reviewed. An important feature of both materials is given by their strong sensitivity to thermal processing: the free carrier concentration and the absorption spectra drastically vary as a function of annealing temperature, duration and ambient. The possible causes will be discussed.

Coffee break

O 13.4 Mon 16:30 H2
Surface structure of metal oxides via Fast Atom Diffraction — •Marco Busch[1], Eric Meyer[1], Jan Seifert[1], Helmut Winter[1],

Klaus Irmscher[2], Zbigniew Galazka[2], and Roberto Fornari[2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstrasse 15, D-12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Strasse 2, D-12489 Berlin, Germany

Fast light atoms (H and ^{4}He) and molecules (H_2) with energies from 200 eV up to several keV are grazingly scattered from clean and flat surfaces. For scattering along low-indexed axial channels, we observe defined diffraction patterns in the angular distributions of scattered projectiles, which can be ascribed to Fast Atom Diffraction (FAD) with de Broglie wavelengths as low as about 10^{-3} Å. As example, we have investigated the quantum scattering from the cleaved (100) surface of a Ga_2O_3 single crystal, grown by the Czochralski method following by in situ annealing. The splittings of Bragg peaks and their intensity modulations were so far exploited to deduce information on the arrangement of atoms in the topmost surface layer. Furthermore, diffraction effects were present in the regime of surface channeling, where quantum scattering is considered for the motion parallel to the surface. For the $Al_2O_3(11\bar{2}0)$ surface we found, that beside the *normal coherence* also the *longitudinal coherence* is preserved, so that *Laue circles* are observed. Then, quantum scattering from surfaces gives rise to interesting features and enhances the resolution of FAD by one order of magnitude. As example, we have resolved the (12x4) superstructure on the $Al_2O_3(11\bar{2}0)$ surface obtained after annealing to about 2000 K.

Topical Talk O 13.5 Mon 16:45 H2

Development of gallium oxide power devices — •Masataka Higashiwaki[1,2], Kohei Sasaki[1,3], Akito Kuramata[3], Takekazu Masui[4], and Shigenobu Yamakoshi[3] — [1]National Institute of Information and Communications Technology, Koganei, Tokyo, Japan — [2]JST PREST, Chiyoda, Tokyo, Japan — [3]Tamura Corporation, Sayama, Saitama, Japan — [4]Koha Co., Ltd., Nerima, Tokyo, Japan

Gallium oxide (Ga_2O_3) has excellent material properties for power device applications represented by the extremely large breakdown field of 8 MV/cm due to a large band gap of 4.8–4.9 eV. Another important feature in industry is that large single-crystal β-Ga_2O_3 bulks can be fabricated with melt-growth methods. We recently succeeded in fabricating Ga_2O_3 metal-semiconductor field-effect transistors (MESFETs) and Schottky barrier diodes (SBDs) on single-crystal β-Ga_2O_3 substrates by using newly developed technologies for making single-crystal substrates, growing conductivity-controlled epitaxial films, and fabricating devices. The MESFETs exhibited excellent device characteristics including an off-state breakdown voltage (V_{br}) over 250 V, an extremely low leakage current (several μA/mm), and a high on/off drain current ratio of around 10,000. The SBDs also showed good characteristics such as an ideal factor very close to 1.0 and a high reverse V_{br}. These results indicate that Ga_2O_3 have comparable or even more potential than Si and typical widegap semiconductors SiC and GaN for power device applications.

O 13.6 Mon 17:15 H2

Structural, optical and electrical properties of Si-doped β-β-Ga_2O_3 thin films — •Stefan Müller, Holger von Wenckstern, Florian Schmidt, Daniel Splith, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

The wide bandgap oxide semiconductor β-Ga_2O_3 ($E_g = 4.9$ eV at room temperature) is a promising material for realization of transparent optoelectronics like FETs [1] or solar-blind photodetectors.

In this contribution we present structural, optical and electrical properties of 1% SiO_2-doped β-Ga_2O_3 thin films grown by pulsed-laser deposition (PLD) on *c*-plane sapphire substrates. The oxygen partial pressure was set between 3×10^{-4} and 0.024 mbar and the substrate temperature between 570°C and 730°C. The thin films are ($\bar{2}01$)-oriented if grown at low oxygen partial pressures and high temperatures. At a growth temperature of 730°C and for oxygen partial pressures above 10^{-3} mbar additional orientations are visible in the XRD pattern. The transmissivity between 1100 nm and 280 nm is in the range of 80% for most investigated samples. However, the optical bandgap increases from 4.7 eV (0.04 mbar) to 4.9 eV (3×10^{-4} mbar) with decreasing oxygen partial pressure. The maximal conductivity and electron mobility of our thin films is in the range of 20 S/m and 0.15 cm^2/Vs, respectively.

[1] M. Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012).

O 13.7 Mon 17:30 H2

Schottky contacts on β-Ga_2O_3 thin films grown by pulsed laser deposition — •Daniel Splith, Stefan Müller, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

A promising oxide semiconductor for high power electronics and transparent optoelectronic devices is β-gallium oxide (Ga_2O_3) with a band gap of about 4.9 eV. We have investigated the preparation and the properties of Schottky contacts (SCs) on Ga_2O_3 thin films. The thin films were grown from a Ga_2O_3 target with 1% SiO_2 on c-sapphire substrates using pulsed-laser deposition at an oxygen pressure of 10^{-3} mbar. The ohmic contacts were fabricated by thermal evaporation of Ti and Al as reported in [1]. Subsequently, we prepared SCs by normal and reactive DC sputtering of metals like Nb, W or Cu. The $I-V$ characteristics of such SCs showed rectification ratios up to 8 orders of magnitude for some of the Nb contacts. The dominant current transport mechanism is thermionic emission. From fits we determined ideality factors n down to 1.15 for the best W contacts and barrier heights Φ_B up to 1.2 eV for the best Cu contacts. Temperature dependent $I-V$ measurements yielded a linear dependence of Φ_B and $\frac{1}{n}-1$ on the inverse temperature in accordance to the theory of thermionic emission in the presence of a laterally inhomogeneous barrier. E. g. the mean barrier height $\overline{\Phi}_B$ for the Cu contacts is determined to be 1.6 eV with a standard deviation σ_Φ of 0.17 eV.

[1] E. G. Villora *et al.*, Appl. Phys. Lett. 92, 202118 (2008)

Coffee break

O 13.8 Mon 18:00 H2

Printed, high performance inorganic oxide transistors from halide precursors — •Suresh Kumar Garlapati[1,2], Nilesha Mishra[1], Ramona Hahn[1], Simone Dehm[1], Robert Kruk[1], Subho Dasgupta[1], and Horst Hahn[1,2,3] — [1]Institute for nanotechnology, Karlsruhe institute of technology(KIT) ,Eggenstein, Germany — [2]KIT-TUD Joint research laboratory nanomaterials, TU Darmstadt, Darmstadt, Germany — [3]Center for functional nanostructures, KIT, Germany

Ink-jet printed field-effect transistors (FETs) are recently of great interest for large area electronics; especially when they exhibit high field-effect mobility. The importance of such devices increases even further when they are operated with very low voltages and compatible to portable electronic applications. However, examples of low voltage driven, high mobility FETs that are scalable for high volume production is scarce in the literature. Here, we report ink-jet printed, halide precursor based extremely high mobility oxide (In2O3) FETs that are gated with composite solid polymer electrolytes to limit the operation voltage to 1 V. The printed precursors have been annealed at different temperatures (573-773 K) and as a result devices have shown little dissimilar performance depending on the degree of crystallization and size of crystallites. Nevertheless, the performance for the lowest temperature annealed devices (573 K) has also been quite outstanding; device mobility close to 50 cm^2V^-1s^-1 and On/Off ratio in excess of 10^5 is noted. The achieved field-effect mobility ensures high semiconductor quality and excellent semiconductor/dielectric interface.

Topical Talk O 13.9 Mon 18:15 H2

Surface electron accumulation layers in oxide semiconductors — •Tim Veal — University of Liverpool, Liverpool, UK

In contrast to the electron depletion at the surface of almost all n-type semiconductors, electron accumulation has long been known to occur at ZnO surfaces. It has recently been found to be characteric of several other oxide semiconductors, including CdO [1,2], In_2O_3 [3] and SnO_2. They all have a significant size and electronegativity mismatch between their cation and anion. As a result, they have a particularly low Γ-point conduction band minimum which is ultimately responsible for the propensity for electron accumulation. As well as the existence of an electron-rich layer, it has been found, using angle-resolved photoemission spectroscopy (ARPES), to be quantized into 2D subbands [1]. Moreover, the conventional one-electron picture of surface space-charge in semiconductors is shown to be inconsistent with the electronic structure observed directly from ARPES, indicating that many-body interactions play a large role in the surface electronic properties of these oxides. Such interactions lead to a depth-dependent shrinkage of the semiconductor band gap, resulting in a surface band gap which differs from the bulk value [1]. The most recent studies have focussed on the influence of depositing alkali metals onto these surfaces. Many

collaborators are acknowledged for samples and ARPES expertise.
[1] P. D. C. King, T. D. Veal *et al.*, PRL **104**, 256803 (2010); [2] P. D. C. King, T. D. Veal *et al.*, PRB **79**, 035203 (2009); [3] P. D. C. King, T. D. Veal *et al.*, PRL **101**, 116808 (2008)

O 13.10 Mon 18:45 H2

Surface and bulk derived in-gap states of In_2O_3 single crystals — •Dorothee Braun[1], Valentina Scherer[1], Christoph Janowitz[1], Zbigniew Galazka[2], and Recardo Manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

The influence of intrinsic point defects on the electronic structure of n-type In_2O_3 single crystals grown by two methods, namely chemical vapor transport (CVT) and melt growth, was examined by two different spectroscopic methods. First, with scanning tunneling spectroscopy (STS), a very surface sensitive technique for measuring the local density of states (LDOS). So far not resolved states within the fundamental band gap have been observed. The gap states have been studied for different crystals and after several temper treatments in oxygen. Second, low-energy angular-resolved photoemission spectroscopy (low-e ARPES) at $h\nu = 9$ eV photon energy has been used to investigate the gap states in the bulk. In contrast to conventional ARPES at typical VUV we were now able to resolve individual emissions of the gap states as well as their momentum dependence. The spectroscopic results will be compared to state of the art DFT-calculations revealing the origin of the gap states in In_2O_3 to be due to oxygen vacancies as well as indium and oxygen interstitials.

O 13.11 Mon 19:00 H2

Electron transport in molecular-beam-epitaxy-grown SnO_2 and In_2O_3 films: Doping, defects, and the surface — •Oliver Bierwagen[1,2], Natalie Preissler[1], Takahiro Nagata[2,3], Mark E. White[2], Min-Ying Tsai[2], and James S. Speck[2] — [1]Paul-Drude-Institut, Berlin, Germany — [2]University of California, Santa Barbara, USA — [3]National Institute for Material Science, Tsukuba

Electron transport and its control are key issues for the application of semiconducting oxides in (opto)electronic devices. To this end, the electron transport in unintentionally- and intentionally doped, high quality, molecular-beam-epitaxy-grown tin oxide (SnO_2) and indium oxide (In_2O_3) films is reviewed.[1] Comparably high mobilities indicate high purity and quality.[2] The resistivity was successfully varied over more than seven orders of magnitude from a transparent conducting oxide-like conductivity by donor doping up to the semi-insulating range (but no p-type conductivity) by acceptor doping.[3,4] Oxygen-related defects play a critical role in In_2O_3.[2, 4] A surface electron accumulation layer is present in both oxides.[5,6] While it strongly influences contact properties,[6,7] its conductance is negligible.[3,6]
[1] O. Bierwagen et al.*Chapter 15 - MBE of transparent semiconducting oxides* in *Molecular Beam Epitaxy*, Elsevier Oxford (2012).
[2] O. Bierwagen and J.S. Speck, Appl. Phys. Lett. 97, 072103 (2010).
[3] O. Bierwagen et al., J. Mater. Res. 27, 2232 (2012).
[4] O. Bierwagen and Speck, Appl. Phys. Lett. 101, 102107 (2012).
[5] T. Nagata et al., Appl. Phys. Lett. 98, 232107 (2011).
[6] O. Bierwagen et al., Appl. Phys. Lett. 98, 172101 (2011).
[7] O. Bierwagen et al., Appl. Phys. Express 2, 106502 (2009); T. Nagata et al. J. Appl. Phys. 107, 033707 (2010).

Concluding remarks

O 14: Topological Insulators 2 (jointly with DS, HL, MA, TT)

Time: Monday 15:00–18:00 Location: H10

Invited Talk O 14.1 Mon 15:00 H10

The THz response of topological insulator surface states — •N. Peter Armitage — The Institute of Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

Topological insulators (TIs) are newly discovered states of matter characterized by an *inverted* band structure driven by strong spin-orbit coupling. One of their most touted properties is the existence of robust "topologically protected" surface states. I will discuss what topological protection means for transport experiments and how it can be probed using the technique of time-domain THz spectroscopy applied to thin films of Bi_2Se_3. By measuring the low frequency optical response, we can follow their transport lifetimes as we drive these materials through instabilities either by doping through a quantum phase transition into a topologically trivial regime or by reducing the film thickness. I'll also discuss our work on the magnetic field dependence of the Kerr rotation in Bi_2Se_3, where we find an unprecedentedly large value of the angle of rotation of reflected light, which is due to the cyclotron resonance of the 2D Dirac fermions.

15 min. break

O 14.2 Mon 15:45 H10

Peierls dimerization at the edge of 2D topological insulators? — •Gustav Bihlmayer[1], Hyun-Jung Kim[2], Jun-Hyung Cho[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics and Research Institute for Natural Sciences, Hanyang University, Seoul, Republic of Korea

Edge states of two-dimensional topological insulators (2D-TIs) attracted considerable interest as they support dissipationless spin-currents. Recently, it was proposed that the zigzag-edge of a Bi(111) bilayer, identified as a 2D-TI [1,2], is unstable with respect to a Peierls dimerization [3], a phenomenon that occurs quite general in one-dimensional structures. This proposal was based on an *ab initio* investigation without taking spin-orbit coupling (SOC) into account. We investigate the effect of SOC on the atomic structure of zigzag Bi(111) and Sb(111) nanoribbons. Although we find that edge-reconstructions can influence the number of conductive channels, we conclude that the topological protection of the states in the Bi ribbon actually prevents the Peierls mechanism to get effective, since the opening of a Peierls gap at the zone boundary is forbidden by time-reversal symmetry. We compare the situation to the Sb structure, but also in the topologically trivial case of the Sb(111) bilayer ribbon we find a suppression of the dimerization due to SOC effects.

[1] S. Murakami, Phys. Rev. Lett. 97, 236805 (2006) [2] M. Wada et al., Phys. Rev. B 83, 121310(R) (2011) [3] L. Zhu et al., J. Phys. Chem. C 114, 19289 (2010)

O 14.3 Mon 16:00 H10

Engineering quantum anomalous Hall (QAH) phases with orbital and spin degrees of freedom — •Hongbin Zhang, Frank Freimuth, Gustav Bihlmayer, Marjana Ležaić, Stefan Blügel, and Yuriy Mokrovsov — Peter Grünberg Institut and Institute for Advanced Simulation, FZJ and JARA, 52425 Jülich, Germany

Combining tight-binding models and first-principles calculations, we demonstrate that under external exchange fields, non-zero Chern numbers and nontrivial QAH effects can be induced by on-site spin-orbit coupling (SOC) in buckled honeycomb lattices with *sp* orbitals. In the Haldane model [1], the occurrence of the QAH effect is attributed to complex valued next-nearest-neighbor hopping matrix elements. Detailed analysis of a generic tight binding model reveals that there exist different mechanisms giving rise to complex hoppings, utilising both orbital and spin degrees of freedom of electrons on a lattice. Furthermore, it is shown that in Bi- or Sb(111) bilayers [2], different topological phases exist as function of the magnitude of SOC and external exchange fields. These phases are characterised using Chern and spin Chern numbers [3] in combination with transverse charge and spin conductivities. At last, we show that introducing ferromagnetic dopants provides a practical way to induce nontrivial topological phases, whereas the physics is altered due to partially filled *d* states around the Fermi energy. – Support by Helmholtz Young Investigators Group Programmes VH-NG-409 and -513 is acknowledged.

[1] F.D.M. Haldane, PRL **61**, 2015 (1988). [2] H. Zhang, *et al.*, PRB **86**, 035104 (2012). [3] E. Prodan, PRB **83**, 195119 (2011).

O 14.4 Mon 16:15 H10

Prediction of weak topological insulators in layered semiconductors — •Binghai Yan[1,2], Lukas Müchler[1,2], and Claudia

Felser[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden — [2]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg University of Mainz, 55099 Mainz

We report the discovery of weak topological insulators by ab initio calculations in a honeycomb lattice. We propose a structure with an odd number of layers in the primitive unit cell as a prerequisite for forming weak topological insulators. Here, the single-layered KHgSb is the most suitable candidate for its large bulk energy gap of 0.24 eV. Its side surface hosts metallic surface states, forming two anisotropic Dirac cones. Although the stacking of even-layered structures leads to trivial insulators, the structures can host a quantum spin Hall layer with a large bulk gap, if an additional single layer exists as a stacking fault in the crystal. The reported honeycomb compounds can serve as prototypes to aid in the finding of new weak topological insulators in layered small-gap semiconductors.

O 14.5 Mon 16:30 H10

Dirac States in a Novel Topological Insulator: Epitaxial alpha-Tin Layers on Indium Antimonide — •J. Schäfer[1], A. Barfuss[1], G. Bihlmayer[2], D. Wortmann[2], L. Dudy[1], P. Höpfner[1], A. Bostwick[3], E. Rotenberg[3], and R. Claessen[1] — [1]Phys. Inst., Universität Würzburg, D — [2]Peter Grünberg Inst. and Inst. Adv. Sim., FZ Jülich, D — [3]Lawrence Berkeley Nat. Lab., USA

This study addresses a new material realization of a topological insulator (TI) thus far only proposed theoretically, which is formed by α-Sn in the diamond lattice on InSb substrates. The epitaxial growth opens various pathways to access and manipulate the topological surface state (TSS). This includes the evolution of the Dirac bands as a function of thickness, or surface coating layers which alter the spin-orbit interaction. Interestingly, the TI band properties are closely related to that of strained HgTe, for which the Quantum Spin Hall effect was demonstrated.

Here we report on the electronic structure of α-Sn(001) based on angle-resolved photoemission (ARPES), complemented by density functional theory (DFT). We observe the formation of a clearly pronounced Dirac cone. The Fermi level in ARPES is located close to the Dirac point. Its position can be controlled by dopants, which allows to adjust the Fermi level crossings of the TSS. The Dirac cone is discernible down to bulk band energies, and its constant energy surfaces seemingly reflect the lattice symmetry. The experimental findings are consistent with DFT calculations including spin-orbit interaction, which document the formation of a TSS.

O 14.6 Mon 16:45 H10

Observation of terahertz photocurrents in the topological insulator Bi_2Se_3 — •Lukas Braun[1], Luca Perfetti[2], Martin Wolf[1], and Tobias Kampfrath[1] — [1]Physikalische Chemie, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Laboratoire des Solides Irradiés, Ecole Polytechnique, Palaiseau cedex, France

Recent experiments have indicated that optical excitation of topological insulators (TIs) with circularly polarized light can induce spin-polarized electron currents along the TI surface. The direction of this photocurrent can be controlled by varying the circular polarization of the driving light from right- to left-handed. So far, only DC photocurrents have been detected [J. W. McIver *et al.* Nature Nanotechnology **7**, 96 (2012)]. Since electrons moving through a solid typically undergo scattering on sub-picosecond time scales, it is highly desirable to generate and detect TI photocurrents with femtosecond time resolution.

Here, we drive ultrashort current bursts in n-doped Bi_2Se_3 by excitation with a laser pulse (10fs, 800nm, 10nJ). The photocurrent gives rise to the emission of a terahertz (THz) electromagnetic pulse whose transient electric field $E(t)$ is detected by means of electro-optic sampling with a time resolution of 10fs. We observe extremely broadband THz emission covering the range from 10 to 30THz, and the THz intensity is found to depend strongly on the helicity of the pump pulses. A method is presented that allows us to extract the transient current $j(t)$ from the measured $E(t)$. We finally discuss the origin of $j(t)$ and implications for the dynamics of photoexcited TI electrons.

O 14.7 Mon 17:00 H10

Static screening properties of topologically protected surface states — •Daniel Wortmann, Gustav Bihlmayer, Yuriy Mokrousov, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The electrons occupying surface states of topological insulators (TI) provide charges that can screen electric fields applied perpendicular to the surface. Being a very basic phenomenon, its realistic description is rather difficult: model approaches fail to provide quantitative results while DFT calculations of insulating slabs with external electric fields suffer from difficulties arising from the incomplete screening of the field inside the slab.

We demonstrate that the embedded Green function method [1,2] can be utilized to investigate the effects of an applied field on the surface states. Our approach describes the formation of surface states in terms of their scattering properties at the semi-infinite bulk states by means of a generalized logarithmic derivative. Besides discussing the underlying idea of this elegant theoretical tool and its application to prototypical topological insulators, we present a comparison of the expected screening effects seen in a topological insulator with those in a topological material.

[1] see http://www.flapw.de for details of the code

[2] D. Wortmann, H. Ishida, S. Blügel, Phys. Rev. B **65**, 165103 ('02)

O 14.8 Mon 17:15 H10

Topological phases of spin chains — Kasper Duivenvoorden and •Thomas Quella — Universität zu Köln, Institut für Theoretische Physik, Köln, Deutschland

The Haldane phase of one-dimensional $S = 1$ spin chains with $SU(2)$ symmetry is one of the first topological states of matter. In particular, it features a bulk-boundary correspondence, with $S = 1/2$ degrees of freedom emerging at the boundaries of the system. Moreover, it exhibits a diluted anti-ferromagnetic order which can be measured using a non-local string order parameter. With the prospect of being able to simulate spin chains with $SU(N)$ symmetry in the laboratory using ultracold earth-alkaline atoms it is a natural and interesting question whether similar topological phases also exist beyond $N = 2$.

In a recent paper we have shown that this is indeed the case. More precisely, spin chains with $SU(N)$ symmetry allow for up to N different topological phases, $N - 1$ of which are topologically non-trivial. These phases exhibit topological order that is reflected in a specific entanglement pattern resulting from the matrix product state representation of the corresponding ground state wave function. It may be detected using a non-local string order parameter which characterizes each of the N phases unambiguously. Analytical and numerical results confirm that our order parameter may be used to extract a quantized topological invariant.

O 14.9 Mon 17:30 H10

Strongly-correlated topological semiconductors — •Stanislav Chadov[1], Claudia Felser[1], Leon Petit[2], Hubert Ebert[3], and Jan Minár[3] — [1]MPI-CPFS Dresden — [2]STFC Daresbury Laboratory, UK — [3]LMU München

Using the fully-relativistic Green's function formalism we analyze the electronic structure topology in series of the heavy rock-salt type semiconductors PuX, SmX (X=Te, Se, S). Due to the partial filling of their f-shells, these materials exhibit strong dynamical correlations which destroy the Bloch-like eigenstates. Thus, the usual analysis based on the symmetry of the eigenstates cannot be applied. Here we recall the adiabatic approach, which allows to analyze the topology based on a purely bulk information disregarding the Bloch or localized character of the electronic states. The dynamical correlations were treated within the DMFT scheme implemented in the framework of the SPR-KKR Green's function method.

O 14.10 Mon 17:45 H10

Correlation between linear Magnetoresistance and Mobility of Heusler Topological Insulators — •C. Shekhar, A. K. Nayak, S. Ouardi, G. H. Fecher, and C. Felser — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Topological insulators (TIs) are a class of quantum materials and belong to a new state of matter with topologically protected gapless Dirac fermionic states. Among the TIs series Heusler compounds are promising candidates for the nanoelectronic devices. If these compounds contain heavy metals (Au, Pb, Pd, Pt, Sb and Bi) and a lanthanide element then they exhibit extraordinary physical properties including *zero band gap*. Generally, gapless compounds show high mobility, where no threshold energy is required to conduct carriers from occupied states to empty states. Very recently, the exciting discovery of graphene is an example of high-mobility compounds due to its linear dispersion of the bands, where charge carriers behave like massless particles. However, the Heusler TIs having *zero band gap* are also expected to show high mobility. The Heusler TIs also exhibit nonsaturating and positive magnetoresistance, that shows systematic variations with temperature. The best fitting of observed MR is found with the combination of linear and quadratic field dependence and may be written in form of a quadratic equation: MR $= a|B| + (b/2)B^2$, where B is applied field. It is clear that this MR originates from the contribution of both linear and parabolic terms. The parabolic term is well known and comes from the Lorentz force, while the origin of the linear MR is intriguing.

O 15: Focussed Session: Correlations in Topological Bands (jointly with DS, HL, MA, and TT)

Topological ideas have been among the most profound recent additions to the field of condensed matter physics, and they have provided some of the most unexpected new developments, most recently through the proposed existence of fractional Chern insulators: these are lattice systems in which fractional quantum Hall physics occurs in partially filled non-dispersive topological “Chern” bands. Our ability to create such environments is central to advancing the understanding of correlated electron physics.

This session focuses on the twin aspects of the new physics that can be found in such settings on one hand, and recent progress towards realizing such settings on the other. It contains theoretical and experimental contributions, from nano-, semiconductor and cold atomic physics.

Organizer: Roderich Moessner (MPI PKS, Dresden)

Time: Monday 15:00–17:45 Location: H20

Invited Talk O 15.1 Mon 15:00 H20

Designer Dirac Fermions, Topological Phases, and Gauge Fields in Molecular Graphene — •Hari C. Manoharan — Dept. of Physics, Stanford University, Stanford, California 94305, USA

Using low-temperature scanning tunneling microscopy and spectroscopy, we show the emergence of Dirac fermions in a fully tunable condensed-matter system—molecular graphene—assembled via atomic manipulation of a conventional two-dimensional electron system in a surface state. We embed, image, and tune the symmetries underlying the two-dimensional Dirac equation into these electrons by sculpting the surface potential with manipulated molecules. By distorting the effective electron hopping parameters into a Kekulé pattern, we find that these natively massless Dirac particles can be endowed with a tunable mass engendered by the associated scalar gauge field, in analogy to the Higgs field. With altered symmetry and texturing of the assembled lattices, the Dirac fermions can be dressed with gauge electric or magnetic fields such that the carriers believe they are in real fields and condense into the corresponding ground state, as confirmed by tunneling spectroscopy. Using these techniques we ultimately fabricate a quantum Hall state without breaking time-reversal symmetry, in which electrons quantize in a gauge magnetic field ramped to 60 Tesla with zero applied laboratory field. We show that these and other chiral states now possible to realize have direct analogues in topological insulators, and can be used to guide or confine charge in nontrivial ways [1].

[1] Gomes et al., Nature **483**, 306–310 (2012).

Invited Talk O 15.2 Mon 15:30 H20

Fractional Topological Insulators — •Claudio Chamon[1], Christopher Mudry[2], Titus Neupert[2], and Luiz Santos[3] — [1]Boston University — [2]Paul Scherrer Institute — [3]Perimeter Institute

The prediction and experimental discovery of topological band insulators and topological superconductors are recent examples of how topology can characterize phases of matter. In these examples, electronic interactions do not play a fundamental role. In this talk we shall discuss cases where interactions lead to new phases of matter of topological character. Specifically, we shall discuss fractional topological states in lattice models which occur when interacting electrons propagate on flattened Bloch bands with non-zero Chern number. Topologically ordered many-particle states can emerge when these bands are partially filled, including a possible realization of the fractional quantum Hall effect without external magnetic fields. We also discuss the importance of geometric band attributes to stabilize certain fractional states, highlighting the importance of geometry and not just topology for reaching fractional states of matter.

Topical Talk O 15.3 Mon 16:00 H20

Hierarchy of Fractional Chern Insulators and Competing Compressible States — •Andreas Läuchli — Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Österreich

The recent engineering of simple tight binding models harboring flat bands with non-zero Chern number calls for a detailed study of the possible many-body phases occurring in partially filled Chern bands and their analogies and differences compared to the continuum Landau level problem. We first report the numerical phase diagram for a flat Chern band with $C = 1$ on the checkerboard lattice, where we find hierarchy multiplets of incompressible states at various fillings ν These are accounted for by an analogy to Haldane pseudopotentials extracted from an analysis of the two-particle problem. Important distinctions to standard fractional quantum Hall physics are striking: absent particle-hole symmetry in a single band, an interaction-induced single-hole dispersion appears, which perturbs and eventually destabilizes incompressible states as ν increases [1]. In second study we investigate the occurrence of fractional Chern insulating phases in a series of bands with higher Chern numbers $C = N > 1$. We find compelling evidence for a series of stable states at $\nu = 1/(2N + 1)$ for fermions as well as bosonic states at $\nu = 1/(N + 1)$. By examining the topological ground state degeneracies and the excitation structure as well as the entanglement spectrum, we conclude that these states are Abelian [2].

[1] A. M. Läuchli, Z. Liu, E.J . Bergholtz, and R. Moessner, arxiv:1207.6094 (2012)

[2] Z. Liu, E. J. Bergholtz, H. Fan, and A. M. Läuchli, Phys. Rev. Lett. **109**, 186805 (2012)

15 min. break

Topical Talk O 15.4 Mon 16:45 H20

Designing Topological Bands for Ultracold Atomic Gases — •Nigel Cooper — Cavendish Laboratory, University of Cambridge, UK

One of the most important techniques in the ultracold atom toolbox is the optical lattice: a periodic scalar potential formed from standing waves of light. Optical lattices are central to the use of atomic gases as quantum simulators, and allow the exploration of strong-correlation phenomena related to condensed matter systems. I shall describe how to design new forms of optical lattice - so-called “optical flux lattices” - in which optically dressed atoms experience a periodic effective magnetic flux with high mean density. Optical flux lattices have narrow energy bands with nonzero Chern numbers, analogous to the Landau levels of a charged particle in a uniform magnetic field. These lattices will greatly facilitate the achievement of the quantum Hall regime for ultracold atomic gases.

Topical Talk O 15.5 Mon 17:15 H20

Probing Topological Bloch Bands Using Ultracold Quantum Gases — •Immanuel Bloch — Max-Planck Institut für Quantenoptik, Garching, Germany — Ludwig-Maximilians Universität, München, Germany

Over the past years, ultracold quantum gases have emerged as highly controllable testbeds for probing fundamental condensed matter phenomena. In my talk, I will show how strong effective magnetic fields can be realized for neutral atoms held in an especially engineered optical lattice potential. The effective field strengths that can be reached, are 10-100 times larger than what can be achieved even with the strongest magnets in real material systems, allowing one to take the artificial quantum matter into a new parameter regime. Furthermore, I will show how by carrying out matter wave interferometry within the Bloch bands, we have been able to measure the Zak phase - the Berry phase in one dimension - and to directly determine topological invariants. As an example, I will present results for the celebrated Su-Schrieffer-Heeger model of polyacetylene that can be modelled by using optical superlattice potentials.

O 16: Magnetic Excitations: from surfaces down to adatoms (jointly with MA)

Organizer: Stefan Blügel (Forschungszentrum Jülich)

In recent years, major advancements have been made in the study of collective, localized, and discrete excitations in itinerant nanomagnets and atomic quantum magnets. This progress has been triggered by the development of spin-polarized electron energy loss spectroscopy (SPEELS) and by low-temperature scanning probe techniques (STM). These tools probe inelastic spin-dependent phenomena and moved the investigation of inelastic magnetic effects to the forefront of research in nanomagnets. Challenged by these experiments, new theoretical approaches have been developed, e.g. based on time-dependent density functional theory and many-body perturbation theory. In this session, we focus on a variety of new physics in this area of research. We start from the collective excitations in low-dimensional films as measured with SPEELS and inelastic STM and then move to systems of small adclusters and adatoms.

Time: Monday 15:00–17:30 Location: H23

Topical Talk O 16.1 Mon 15:00 H23
Tailoring magnetic excitations in low-dimensional ferromagnets — •Khalil Zakeri Lori — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We present a summery of our recent results on elementary magnetic excitations (magnons) in ultrathin ferromagnets. Terahertz magnons in ultrathin Fe(100), Fe(110) and Fe(111) films, grown on different surfaces, are probed by means of spin-polarized high resolution electron energy-loss spectroscopy. The key properties of magnons such as their dispersion relation and lifetime are measured over the entire Brillouin zone. It is demonstrated that these properties depend strongly on the atomic structure of the films as well as the degree of electronic hybridization with the substrate. We discuss how the complexity of the electronic structure, degree of electronic hybridization and the contribution of different orbitals to the exchange interaction can lead to unexpected behavior of magnon energies. The lifetime of terahertz magnons is found to be a few tens of femtoseconds at low wave vectors, which reduces significantly as the wave vector approaches the Brillouin zone boundary. Based on our results we comment on the damping mechanism of terahertz magnons. Finally, we introduce a way of tailoring the properties of terahertz magnons by engineering the electronic structures.

Topical Talk O 16.2 Mon 15:30 H23
Theory of spin waves in ultrathin ferromagnetic films — •Roberto Muniz and Antonio Costa — Instituto de Fisica, Universidade Federal Fluminense,Niteroi, RJ 24210-346, Brazil

We review our theoretical studies of spin dynamics in ultrathin ferromagnetic films adsorbed on metallic substrates. Our approach is based on a realistic description of the electronic structure for the substrate/adsorbate combination. Ferromagnetism in the film is driven by on site Coulomb interaction between the d electrons treated in mean field theory, and the spin wave excitations are described by the transverse spin dynamic susceptibility, which is calculated within the random phase approximation. We find the lifetimes of short-wavelength spin excitations in such systems are very short due to their decay to Stoner excitations, in accordance with spin-polarized electron energy-loss spectroscopy (SPEELS) data. We also discuss the influence of spin-orbit coupling on the spin-wave excitation spectra and find that our theory accounts for asymmetries seen in SPEELS studies of spin waves in the bilayer of Fe on W(110).

Topical Talk O 16.3 Mon 16:00 H23
Magnetic excitations in all metallic nanostructures — •Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

The spins in magnetic nanostructures can be excited, when passing an electric current through them. In the inelastic scattering events, the spin of a hot electron of the current provided by a scanning tunneling microscope may be flipped and angular momentum is transferred to the magnetic system [1]. We used this technique to determine magnon dispersions and life times in thin itinerant magnetic films [2] and to determine the magnetic anisotropy and exchange coupling in atomically assembled magnetic clusters [3]. Finally, we show that the technique is capable to detect spin flips also in rare earth clusters and that the anisotropy as well as the life times of the states in the 4f-systems require a fully relativistic treatment [4].

[1] T. Balashov et al., Phys. Rev. Lett. 97, 187201 (2006), Phys. Rev. B 78, 174404 (2008). [2] C.L. Gao et al., Phys. Rev. Lett. 101, 167201 (2008). [3] T. Balashov et al., Phys. Rev. Lett 102, 257203 (2009). [4] T. Schuh et al., Phys. Rev. B 84, 104401 (2011), Nano Lett. 12, 4805 (2012).

Topical Talk O 16.4 Mon 16:30 H23
Magnetization dynamics derived from excitations of single magnetic atoms on surfaces — •Alexander Ako Khajetoorians — Hamburg University, Hamburg, Germany

With the development of sub-Kelvin high-magnetic field STM, two complementary methods, namely spin-polarized scanning tunneling spectroscopy (SP-STS) [1] and inelastic STS (ISTS) [2-3], can address single spins at the atomic scale. While SP-STS reads out the projection of the impurity magnetization, ISTS detects the excitations of this magnetization as a function of an external magnetic field. They are thus the analogs of magnetometry and spin resonance measurements pushed to the single atom limit. We have recently demonstrated that it is possible to reliably combine single atom magnetometry with an atom-by-atom bottom-up fabrication to realize complex atomic-scale magnets with tailored properties [4-5]. In this talk, I will address recent developments in probing the spin excitations and magnetization curves of atoms on a multitude of non-magnetic surfaces, and the effects of the electronic structure on the precessional dynamics of the atomic spin. Moreover, I will discuss investigations of the magnetization dynamics [6] of coupled spins as probed with spin-resolved STM techniques and how the relaxation is affected by processes like quantum tunneling and spin-transfer torque. [1] A.A.K., *et al.* , PRL, **106**, 037205 (2011); [2] A. J. Heinrich, *et al.* , Science, **306**, 466 (2004); [3] A.A.K, *et al.* , Nature, **467**, 1084 (2010); [4] A.A.K., *et al.*, Nature Physics, **8**, 497 (2012) [5] A.A.K., *et al.* , Science, **332**, 1062 (2011), [6] A.A.K., *et al.*, Science, in press (2012)

Topical Talk O 16.5 Mon 17:00 H23
Theory of dynamical magnetic excitations in itinerant nanomagnets — •Samir Lounis — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

During the past decades we witnessed an unimaginable progress in the observation and understanding of magnetic structures in nanomagnets. In comparison, our understanding of the dynamics, excitations and switching of magnetism in nanostructures is still in its infancy. In the last years inelastic low-temperature spin-polarised scanning tunneling spectroscopy has been developed and explored producing exciting new insights. In these experiments, the electrons interact with the substrate during the tunneling process, exchange energy and possibly spin angular momentum, leading to inelastic tunneling. To understand, predict and unravel the mechanisms behind these excitations, we developed a method based on first-principles. For instance, during the tunneling process, the dynamical magnetic susceptibility is computed, whose imaginary part gives the density of – , as well as the coupling of tunneling electrons with the spin-excitations that is quantified in terms of a self-energy. An overview of our investigations will be presented: $3d$ adatoms deposited on several metallic surfaces: Cu(100), Cu(111), Ag(111) and Pt(111) with a focus on the impact of adatoms atomic number, nature of the substrate, details of the electronic hybridization as well as the decay of the electronic signal into vacuum.

Work supported by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

O 17: Focussed Session: Frontiers of Electronic Structure Theory II (jointly with HL and TT)

Time: Monday 16:00–19:15 Location: H36

O 17.1 Mon 16:00 H36

Excited States of the divacancy in SiC — •Michel Bockstedte[1], Thomas Garratt[1], and Adam Gali[2] — [1]Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudstr. 7B2, D-91058 Erlangen — [2]Wigner Research Centre for Physics, Hungarian Academy of Sciences, PO Box 49, Budapest 1525, Hungary

The negatively charged nitrogen-vacancy center in diamond has emerged as a candidate for the implementation of a qbit in quantum computing. Silicon Carbide also fullfils necessary conditions[1] which makes it a suitable material for this purpose. With the neutral divacancy it possess a defect center with a high spin ground state, which can be manipulated by spin-resonance techniques.[2] Optical excitation of the triplet ground state and subsequent spin-selective recombination via yet unknown intermediate spin-singlet states enables spin-initialization with M_z=0, which is requisit for a qbit. Here we investigate the excitation spectrum of the divacancy based *ab initio* methods. DFT and TD-DFT calculations[3] reveal a Jahn-Teller effect for the first excited triplet state that is absent for the NV-complex. TD-DFT and an *ab initio* many body hamiltonian nicely reproduce the prominent photoluminescence transitions. The latter method also describes the spin-singlet states. We discuss the defect excitation spectrum in the light of the Jahn-Teller distortion.

[1] J. R. Weber *et al.*, PNAS **107**, 8513 (2010).
[2] F. Koehl *et al.*, Nature **479**, 84 (2011).
[3] A. Gali, phys. status solidi (b) **248**, 1337 (2011).

O 17.2 Mon 16:15 H36

Extending the random phase approximation for electronic correlation energies: The renormalized adiabatic local density approximation — •Thomas Olsen — Technical University of Denmark

The adiabatic connection fluctuation-dissipation theorem with the random phase approximation (RPA) has recently been applied with success to obtain correlation energies of a variety of chemical and solid state systems. The main merit of this approach is the improved description of dispersive forces while chemical bond strengths and absolute correlation energies are systematically underestimated. In this work we extend the RPA by including a parameter-free renormalized version of the adiabatic local density (ALDA) exchange-correlation kernel. The renormalization consists of a (local) truncation of the ALDA kernel for wave vectors $q > 2k_F$, which is found to yield excellent results for the homogeneous electron gas. In addition, the kernel significantly improves both the absolute correlation energies and atomization energies of small molecules over RPA and ALDA. The renormalization can be straightforwardly applied to other adiabatic local kernels.

O 17.3 Mon 16:30 H36

First-principles IXS spectra for TiO_2 and HfO_2 — •Linda Hung and Francesco Sottile — Ecole Polytechnique, Palaiseau, France

Using time-dependent DFT and many-body perturbation theory, we determine the inelastic x-ray scattering (IXS) spectra for bulk TiO_2 and HfO_2. Excitations from valence and semi-core states are modeled, corresponding to transition energies up to 60 eV. By varying momentum transfer, plasmon dispersion can be observed. We characterize differences in the spectra for the rutile, anatase, and brookite polymorphs of TiO_2, as well as the cubic, tetragonal, and orthogonal polymorphs of HfO_2. These spectra are also Fourier transformed, allowing us to image the real-time and real-space electron density response to external perturbations.

O 17.4 Mon 16:45 H36

Linear-scaling time dependent density-functional theory in the linear response formalism — •Tim J. Zuehlsdorff, Nicholas D. M. Hine, James S. Spencer, Nicholas M. Harrison, and Peter D. Haynes — Imperial College London, UK

In recent years, linear-scaling approaches to density-functional theory have enabled the computation of ground-state properties of large nanostructures and biomolecules. While these methods are now well established, the linear-scaling computation of excited state properties via time-dependent density-functional theory (TDDFT) in the linear response regime is less developed.

In this talk we will present an implementation of TDDFT in the linear response formalism, enabling the computation of low-energy optical absorbtion spectra for large molecules and nanostructures. The method avoids any explicit reference to canonical representations of either occupied and unoccupied Kohn-Sham states and thus achieves linear-scaling computational effort with system size. In contrast to conventional localised orbital formulations where a single basis set is used to represent the occupied and unoccupied Kohn-Sham states, we make use of two sets of in-situ optimised localised orbitals, one for the occupied and one for the unoccupied Kohn-Sham space. The double basis set approach avoids known problems of representing the unoccupied space with localised orbitals optimised for the occupied space, while the in-situ optimisation procedure allows for efficient calculations with a minimal set of basis functions. The method is applied to a number of large-scale test systems in order to demonstrate its validity.

O 17.5 Mon 17:00 H36

Dynamical spin and charge excitations with spin–orbit coupling in 3d adatoms on Cu(111) and Pt(111) — •Manuel dos Santos Dias, Benedikt Schweflinghaus, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The presence of spin–orbit coupling has a fundamental impact on the magnetic excitation spectrum: there is a finite gap at zero frequency and spin and charge excitations become coupled. The excitation spectrum is derived from the dynamical magnetic susceptibility of the electronic system, for which we developed a formalism based on Time–Dependent Density Functional Theory, as implemented in the Korringa–Kohn–Rostoker Green function method [1,2]. As an application, we present first–principles calculations of the charge, longitudinal and transverse magnetic excitations of 3d adatoms deposited on the Cu(111) and Pt(111) surfaces. Focus is on the expected spin–charge coupling induced by the the spin–orbit interaction, and on the dynamical anisotropic effects that generalize the familiar magnetic anisotropy.

Work supported by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] S. Lounis, A. T. Costa, R. B. Muniz and D. L. Mills, Phys. Rev. Lett. **105**, 187205 (2010)
[2] S. Lounis, A. T. Costa, R. B. Muniz and D. L. Mills, Phys. Rev. B **83**, 035109 (2011)

O 17.6 Mon 17:15 H36

Beyond the *GW* approximation: a second-order screened exchange correction — •Patrick Rinke[1], Xinguo Ren[1], Noa Marom[2], Fabio Caruso[1], and Matthias Scheffler[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Texas, Austin, USA

Despite the success of the *GW* method in describing the photoemission spectra of solids, molecules and clusters, challenges remain. For aromatic molecules for example absolute as well as relative positions of ionisation energies and affinities are not well reproduced in perturbative G_0W_0 schemes with different starting points as well as in self-consistent *GW* [1], sometimes even giving the wrong orbital order. Motivated by renormalized second-order perturbation theory [2] for the ground-state energy, we propose a second-order screened exchange correction (SOSEX) to the *GW* self-energy. This correction follows the spirit of the SOSEX correction to the random-phase approximation for the electron correlation energy and reduces the self-correlation error. The performance of the *GW*+SOSEX scheme has been benchmarked for a set of molecular systems, including the G2 set, commonly used acceptor molecules, benzene and the azabenzene molecules. We find that the SOSEX correction improves the description of the spectral properties including the orbital order with respect to the different *GW* schemes, highlighting the importance of reducing the self-correlation error. [1] N. Marom *et al.*, arXiv:1211.0416 [2] X. Ren *et al.*, J. Mater. Sci. **47**, 7447 (2012)

O 17.7 Mon 17:30 H36

A strategy for finding a reliable starting point for G_0W_0 demonstrated for molecules — •Thomas Körzdörfer[1] and Noa Marom[2] — [1]Institut für Chemie, Universität Potsdam, D-14476 Potsdam — [2]Center for Computational Materials, Institute of Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX 78712, USA

Many-body perturbation theory in the G_0W_0 approximation is an increasingly popular tool for calculating electron removal energies and fundamental gaps for molecules and solids. However, the predictive power of G_0W_0 for molecules is limited by its sensitivity to the density functional theory (DFT) starting point. In this contribution, the starting point dependence of G_0W_0 is demonstrated for several organic molecules. Analysis of the starting point dependence leads to the development of a non-empirical scheme that allows to find a consistent and reliable DFT starting point for G_0W_0 calculations by adapting the amount of Hartree-Fock-exchange in a hybrid DFT functional. The G_0W_0 spectra resulting from this *consistent starting point (CSP) scheme* [1] reliably predict experimental photoelectron spectra over the full energy range. This is demonstrated for a test set of various typical organic semiconductor molecules.

[1] T. Körzdörfer and Noa Marom, Phys. Rev. B Rapid Communications **86**, 041110 (2012).

O 17.8 Mon 17:45 H36

Electronic properties of isolated and supported organic dyes modeled through the GW method — •Paolo Umari[1], Filippo De Angelis[2], Luigi Giacomazzi[3], Mariachiara Pastore[2], and Stefano Baroni[3] — [1]Dipartimento di Fisica e Astronomia, Università di Padova, Italy — [2]Istituto CNR di Scienze e Tecnologie Molecolari, Perugia, Italy — [3]Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy

The first-principles GW method is used for investigating the electronic levels of isolated and supported dyes for electrochemical solar cells. We consider a set of all-organic dyes, (L0,L2,L3,L4) exhibiting the same donor and anchor groups. First, we calculate the energy levels in the limit of isolated molecules obtaining nice agreement with available experimental photoelectron spectra. Then, we consider the L0 and the L2 dyes while adsorbed on the anatase TiO_2 (101) surface. Also in this case we find good agreement when comparing with available experimental photoelectron spectra. We find that the HOMO -LUMO gap of the dye is reduced with respect to the isolated molecule and that the HOMO level is slightly shifted towards higher energies due to image charge effects. This permits us to derive a simple model for obtaining approximate GW energy levels for the HOMO and the LUMO of the adsorbed molecule and for the valence band maximum and the conduction band minimum of the substrate performing just one complete GW calculation of the isolated molecule and one of the bulk TiO_2 combined with a calculation at the DFT level of the adsorbed molecule complex. In this way, we can investigate larger, more realistic, model structures.

O 17.9 Mon 18:00 H36

Ab-initio description of satellites in semiconductors — •Matteo Guzzo[1,2], Josh J. Kas[3], Lorenzo Sponza[1,2], Christine Giorgetti[1,2], Francesco Sottile[1,2], Debora Pierucci[4], Mathieu G. Silly[4], Fausto Sirotti[4], John J. Rehr[3], and Lucia Reining[1,2] — [1]LSI, Ecole Polytechnique, Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]UW, Seattle, USA — [4]Synchrotron Soleil, Gif-sur-Yvette, France

The GW method from Many-Body Perturbation Theory has been very successful in describing photoemission spectra in a variety of systems. In particular, GW is known to give good quasiparticle properties like band gaps, but it has shown some limitations in the description of complex correlation effects like satellites. Satellite peaks in photoemission come from higher-order excitations and are still poorly studied in the valence bands. In perturbative GW the spectral function can describe additional features beside the quasiparticle peaks, but these satellites are known to be too weak and too low in energy, as it appears from calculations on the Homogeneous Electron Gas and some real materials. Including additional diagrams in the Green's function we obtain an excellent description of satellites series in the test case of bulk silicon, where GW is unable to cope [1]. This approach can be extended to more complex system, i.e. graphite. Using our newly measured XPS valence data, we investigate the effects of anisotropies on satellites and give a prediction on the spectral changes following the transition towards true freestanding graphene. [1] M. Guzzo et al., Phys. Rev. Lett. 107, 166401 (2011)

O 17.10 Mon 18:15 H36

Optical spectra of alkali-metal fluorides — •Christoph Sommer, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany

We have studied the virtue of different approximations for quasiparticle energies in the calculation of optical spectra including excitonic effects by solving the Bethe-Salpeter equation (BSE). To this end, we have computed exemplarily optical spectra of the three alkali-metal fluorides LiF, NaF, and KF using quasiparticle energies resulting from two different approximations of the self-energy operator in Hedin's *GW* approach as well as electronic energies and wave functions obtained by employing self-interaction corrected pseudopotentials. The energetic positions of characteristic peaks in the calculated and measured spectra are in very good agreement when quasiparticle energies are used that result after an update of the screened interaction W on the basis of a preceding G_0W_0 calculation. Additionally, two simple further approximations for one-particle energies that use input either from experiment or from quasiparticle calculations for a small set of wave vectors are included into this investigation.

O 17.11 Mon 18:30 H36

Bethe-Salpeter Equation from many-body perturbation theory — •Tobias Sander, Ronald Starke, and Georg Kresse — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The Green function formalism is a powerful tool to calculate not only electronic structure within the quasi-particle (QP) picture, but it also gives access to optical absorption spectra. Starting from QP energies within the GW method, the polarizability, as central quantity, is calculated from the solution of a Bethe-Salpeter-like equation (BSE). It is usually solved within the Tamm-Dancoff Approximation (TDA) which neglects the coupling of resonant (positive frequency branch) and anti-resonant (negative frequency branch) excitations. In this work we solve the full BSE [1] (beyond TDA) based on self-consistently calculated QP orbitals and energies [2] for typical systems. The dielectric function is averaged over many low dimensional shifted **k**-meshes to obtain **k**-point converged results. We compare the results to recently introduced approximation to the BSE kernel [3]. Additionally, the time-evolution ansatz [4] is employed to calculate the polarizability, which avoids the direct solution of the BSE.

[1] S. Albrecht, L. Reining, R. Del Sole, G. Onida, PRL 80, 4510 (1998)
[2] M. Shishkin, M. Marsman, G. Kresse, PRL 99, 246403 (2007)
[3] L. Reining, PRL 88, 66404 (2002)
[4] W. G. Schmidt, S. Glutsch, P. H. Hahn, F. Bechstedt, PRB 67, 085307 (2003)

O 17.12 Mon 18:45 H36

Acceleration of the response function convergence using the effective energy techniques within the ultrasoft pseudopotential and PAW methods — •Jiří Klimeš and Georg Kresse — Faculty of Physics, University of Vienna, A-1090 Vienna, Austria

Calculations of quasiparticle spectra based on the GW approximation or evaluation of total energies using the RPA method are of a wide interest in the computational materials community. However, their applicability is to a large extent limited by the cost of evaluating the response function or the selfenergy where a large number of unoccupied bands needs to be included. A promising way to speed-up the convergence is to use the resolution of identity and replace the sum over an infinite number of unoccupied states by an effective correction [1,2]. However, the available schemes have been only formulated for norm-conserving pseudopotentials and when applied directly within the ultrasoft pseudopotentials (USPPs) or the PAW method they introduce an error since the correction term doesn't vanish when the number of included bands is increased. Here we present an implementation of the schemes within the formalism of USPPs or the PAW method which gives the proper behaviour of the correction term. We also show how the convergence of the scheme given in [2] can be further improved and discuss the efficiency of the methods for RPA total energy calculations.

[1] F. Bruneval and X. Gonze, PRB **78**, 085125 (2008)

[2] J. A. Berger, L. Reining, and F. Sottile, PRB **82**, 041103(R) (2010); PRB **85**, 085126 (2012)

O 17.13 Mon 19:00 H36

SnO: GW band gap of a van der Waals bonded system — •Kirsten Govaerts[1], Rolando Saniz[2], Bart Partoens[2], and Dirk Lamoen[1] — [1]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium — [2]CMT group, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium

In this work we have investigated the structural and electronic properties of SnO, which is built up by layers kept together by van der Waals (vdW) forces. The combination of a vdW functional (within DFT) and GW calculations leads to accurate values for the c/a ratio and the fundamental band gap. A comparison is made between three starting points for the GW calculation: a regular PBE calculation, one with the vdW effect included, and a hybrid functional calculation. The difference between different levels of self-consistency is also investigated.

O 18: Organic/bio Molecules on Metal Surfaces II

Time: Monday 16:00–19:00 Location: H38

O 18.1 Mon 16:00 H38

Towards a Quantitatively Reliable Modeling of Large Organic Molecules Adsorbing on Metal Surfaces — •David Alexander Egger[1], Yuli Huang[2], Elisabeth Wruss[1], Victor Gonzalo Ruiz[3], Alexandre Tkatchenko[3], Satoshi Kera[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology. — [2]Graduate School of Advanced Integration Science, Chiba University. — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft.

At interfaces in metal-organic hetero-structures a variety of often difficult to quantify interactions such as charge-transfer, polarization, Pauli pushback and van der Waals (vdW) attraction occurs. Such interactions make the identification of the responsible interfacial binding mechanism particularly difficult. We here model a variety of prototypical metal-organic heterostructures including mono- and double-layers of Cu-phthalocyanine (CuPc), a double-layer of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) and CuPc, and non-planar phthalocyanine layers adsorbing on noble-metal surfaces. Using recently developed theoretical tools to properly account for vdW interactions, we achieve remarkable agreement with experiments. Beyond that, we provide atomistic insight into the various processes responsible for the formation of these nanostructures and underline the comparatively large contribution of vdW interactions to the overall binding energies of these systems.

O 18.2 Mon 16:15 H38

Orbital ordering for PTCDA on Ag surfaces — •Martin Willenbockel[1,2], Benjamin Stadtmüller[1,2], Kathrin Schönauer[1,2], Francois C. Bocquet[1,2], Daniel Lüftner[3], Eva M. Reinisch[3], Thomas Ules[3], Georg Koller[3], Christian Kumpf[1,2], Serguei Soubatch[1,2], Peter Puschnig[3], Michael G. Ramsey[3], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Jülich, Germany — [3]Institut für Physik, Karl-Franzens-Universität Graz, 8010 Graz, Austria

The energy alingment of electronic levels for molecules adsorbed on noble metal surfaces was investigated extensively. However, the research was focused mainly on the frontier orbitals located close to the Fermi level, namely the LUMO (lowest unoccupied molecular orbital) and HOMO (highest occupied molecular orbital).

We report a study of PTCDA (3,4,9,10-perylene-tetracarboxylic-dianhydride) adsorbed on the low index Ag surfaces Ag(100), Ag(111) and Ag(110) where the fine structure of the "HOMO-1" resonance was investigated by angle resolved photoemission spectroscopy. Using the orbital tomography approach we found that this resonance consists of 4 close located molecular orbitals [1,2]. The energy ordering of the orbitals is independent from the Ag surface and the molecular superstructure.

[1] P. Puschnig et al., *Phys. Rev. B* **84** 235427 (2011). [2] P. Puschnig et al., *Science* **326** 702 (2009).

O 18.3 Mon 16:30 H38

Orbital tomography: Deconvoluting photoemission spectra of organic molecules — •Sergey Soubatch[1], Martin Willenbockel[1], Benjamin Stadtmüller[1], Kathrin Schönauer[1], Eva Reinisch[2], Thomas Ules[2], Daniel Lüftner[2], Markus Ostler[3], Georg Koller[2], Peter Puschnig[2], Christian Kumpf[1], Mike Ramsey[2], and Stefan Tautz[1] — [1]Peter Grünberg Institut (PGI-3), JARA, Forschungszentrum Jülich, Germany — [2]Institute of Physics, Karl-Franzens University Graz, Austria — [3]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany

The valence bands of organic molecules consist of closely spaced electronic levels, which is often challenging for both theory and spectroscopic experiment. We propose a tomographic method that employs the energy and momentum dependence of photoemission of adsorbed molecules to deconvolute corresponding valence band into individual orbitals beyond the limits of energy resolution.

Photoemission experiments on different ordered monolayer phases of perylene-tetracarboxylic-dianhydride (PTCDA) molecule on low index Ag surfaces were performed at BESSYII storage ring using toroidal electron energy analyzer. For the phases containing molecules nonequivalent either from intermolecular environment or substrate registry point of view, method provides access to electronic properties of either molecule separately. This enables detailed description of site- and orientation-specific bonding of organic molecules at metals, and in so doing, delivers stringent tests for the development of ab-initio electronic structure theory.

O 18.4 Mon 16:45 H38

Spatial distribution of molecular orbitals from angle-resolved photoemission — •Daniel Lüftner[1], Thomas Ules[1], Eva Maria Reinisch[1], Georg Koller[1], Sergey Soubatch[2], F. Stefan Tautz[2], Michael G. Ramsey[1], and Peter Puschnig[1] — [1]Institut für Physik, Karl-Franzens-Universität Graz, Austria — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany

The frontier electronic orbitals of molecules are the prime determinants of the respective compounds' chemical, electronic, and optical properties. Several experimental methods have enabled imaging of molecular orbitals under certain conditions. As has been shown in a number of recent publications, angle-resolved photoemission (ARPES) intensity maps of organic molecular layers are related to the Fourier transform of the initial state molecular orbital. However, the missing phase information impedes the back-transformation of the momentum maps of the orbital into real space. Here, we show how the absent phase information can be retrieved by applying an unbiased, iterative procedure which takes the experimental ARPES maps as input and only assumes spatial confinement of the orbital. Thereby we obtain real-space images of several molecular orbitals for two proto-typical pi-conjugated molecules: the LUMO, HOMO, and HOMO-1 of pentacene, and the LUMO and HOMO of PTCDA. Our technique further emphasizes the capabilities of ARPES looking at spatial distributions of wave functions of adsorbed molecules thereby complementing data obtained from scanning probe methods.

O 18.5 Mon 17:00 H38

Measuring the electron correlation energy between organic

molecules and metal surfaces — •Christian Wagner[1,2], Norman Fournier[1,2], Victor G. Ruiz[3], Alexandre Tkatchenko[3], F. Stefan Tautz[1,2], and Ruslan Temirov[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195, Berlin, Germany

Van der Waals forces have to be considered in any quantitatively correct picture of molecular adsorption. Experimental determination of the energy related to long-range correlation effects is, however, difficult. A measured binding energy is always the result of many contributions, including chemical interactions and Pauli repulsion. Here, we present a measurement of single-molecule adsorption potentials as a function of molecule-surface separation using a frequency modulated atomic force microscope[1,2]. We decompose the different contributions to the potential by their different decay lengths. By investigating molecules with a naphthalene, perylene and terrylene core respectively (NTCDA, PTCDA, TTCDA) on Au(111), we study the dependency of the correlation energy on the size of the aromatic system. We compare the experimentally obtained adsorption potentials to DFT+van der Waals calculations which include dielectric screening within the metal[3].
[1] N. Fournier et al., *Phys. Rev. B* **84**, 035435 (2011)
[2] C. Wagner et al., *Phys. Rev. Lett.* **109**, 076102 (2012)
[3] V. G. Ruiz et al., *Phys. Rev. Lett.* **108**, 146103 (2012)

O 18.6 Mon 17:15 H38

DFTD Calculations on STHM with Xe and CO — •Uwe Friedel and Axel Gross — Theoretical Chemistry, University of Ulm, Germany

The Scanning Tunneling Hydrogen Microscope (STHM) [1] can resolve intramolecular structures of adsorbed molecules and even produce intermolecular contrast along lines of expected hydrogen bondings. The method does not only work with hydrogen, which gave the method the name, but also with other molecules and nobel gas atoms. This talk will present results of dispersion corrected DFT calculations (DFT-D3) with a model tip decorated with a Xe-atom and a CO-molecule.

[1] C. Weiss et al., J. Am. Chem. Soc. 132, 11864 (2010)

O 18.7 Mon 17:30 H38

Single-atom substitution to control the nature of bonding of olympicene on Cu(111) — •Wei Liu[1], Bruno Schuler[2], Nikolaj Moll[2], Leo Gross[2], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]IBM Research – Zurich, 8803 Rüschlikon, Switzerland

The olympicene molecule, consisting of 5 aromatic rings, has been recently synthesized and visualized by atomic force microscopy (AFM) on the Cu(111) surface [1]. Here we show that the substitution of a single atom in the olympicene molecule switches the nature of adsorption from physisorption (olympicene @ Cu), to an intermediate state (olympicene-derived ketone @ Cu), then to strong chemisorption (olympicene radical @ Cu). First-principles calculations using the PBE+vdW$^{\mathrm{surf}}$ method (density-functional theory with screened van der Waals (vdW) interactions [2]), allow us to achieve insights into the stability and electronic structure of complex organic/metal interfaces, and lead to quantitative agreement with atomic force spectroscopy.

[1] http://www-03.ibm.com/press/uk/en/pressrelease/37869.wss.
[2] V. Ruiz *et al.*, PRL **108**, 146103 (2012).

O 18.8 Mon 17:45 H38

Benchmark database of equilibrium geometries and adsorption energies of hybrid organic/metal systems — •Javier Camarillo Cisneros, Wei Liu, Victor G. Ruiz, Nicola Ferri, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der Max Planck Gesellschaft

The adsorption of molecules at transition metal surfaces is important for fundamental and applied surface science studies. Extensive experimental work has been focused on organic/metal interfaces, however, a reliable database that provides accurate binding structures and energetics is still missing. By carefully contrasting a large number of experiments (e.g., normal incidence x-ray standing wave, microcalorimetry, and temperature-programmed desorption), here we create a database that includes more than 20 prototypical adsorption systems, ranging from noble-gas Xe to small/large organic molecules (benzene, naphthalene, C_{60}, PTCDA, etc.) on different metal surfaces. We further study all these interfaces using the PBE+vdW$^{\mathrm{surf}}$ method (density functional theory with screened van der Waals (vdW) interactions [1]), and show that this method yields an agreement of 0.1 Å in equilibrium geometries and 0.1 eV in adsorption energies with state-of-the-art experiments. We assess the quantitative role of vdW interactions for both weakly and strongly adsorbed systems, and show that the constructed database can be used to benchmark the performance of vdW-inclusive first-principles approaches. [1] Ruiz *et al.*, PRL (2012). [2] Liu *et al.*, PRB (2012).

O 18.9 Mon 18:00 H38

Adsorption and thermal polymerization of pentacene on Ir(100) — •Pascal Ferstl, Lisa Lautner, Lutz Hammer, and M. Alexander Schneider — LS f. Festkörperphysik, FAU Erlangen-Nürnberg, Germany

Pentacene molecules were deposited at various temperatures on both the unreconstructed and the quasi-hexagonally reconstructed surface phases of Ir(100) and subsequently thermally processed. On both surfaces the molecules adsorb flat lying, they are immobile at room temperature, but apparently intact. On the fourfold symmetric 1x1 phase there is basically only one particular binding configuration for the molecules, which is either along the [011] or the [$0\bar{1}1$] direction and they randomly assume one of these two (symmetry-equivalent) orientations without any tendency to form ordered domains.

On the one-dimensionally corrugated (5x1) phase the pentacene species deposited at room temperature show three different binding configurations: along the rows of the reconstruction, or inclined by 30° or 90°. Increasing the deposition temperature to above 100°C the adsorption site within the troughs of the reconstruction becomes more and more dominant. For deposition (or annealing) temperatures above 360°C the molecules successively decompose towards a surface carbide. At intermediate temperatures, however, one-dimensional head-to-tail polymerization is found leading to molecular chains of at least double or triple length, which are not observed on the (1x1) phase. This indicates that the substrate reconstruction acts as a template for the molecular reaction scheme at the surface.

O 18.10 Mon 18:15 H38

Nanoscale Control of Molecular Conformation via Tuned Coupling to a Substrate — •Hasmik Harutyunyan[1], Martin Callsen[2], Tobias Allmers[1], Vasile Caciuc[2], Stefan Blügel[2], Nicolae Atodiresei[2], and Daniel Wegner[1] — [1]Westfälische Wilhelms-Universität Münster Wilhelm-Klemm-Str. 10, 48149 Münster, Deutschland — [2]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1) Forschungszentrum Jülich and JARA 52425 Jülich, Deutschland

In recent years the adsorption of organic molecules on noble-metal has shown large interest. Here, it is important to understand the electronic interaction between a gas-phase molecules and the surface, which leads to hybridization and can induce charge transfer. We have investigated the conformation of cyclooctatetraene (COT) on different noble metals by means of low-temperature scanning tunneling microscopy combined with density functional theory. Highly resolved STM images in conjunction with STM simulations enable the unambiguous identification of molecular conformations. The results show, that COT can by stabilized in different conformations by varying its coupling to the noble-metal surface. We find weak physisorption and the tube conformation on Au(111), as know for the gas-phase molecule. On Ag(100) and Cu(100) COT is chemisorbed and planar, as known for charged gas-phase molecules. The conformation of COT can even be manipulated on Au(111) by utilizing nanoscale variations of the molecule-surface interaction. This mechanical and electronic control makes COT an interesting candidate for versatile molecular switches.

O 18.11 Mon 18:30 H38

First Principles Simulations of the Adsorption of Aromatic Molecules on Metallic Surfaces — •Rengin Peköz, Karen Johnston, and Davide Donadio — Max Planck Institute for Polymer Research, Mainz, Germany

Several technologies and applications involve the interaction of aromatic molecules with metal substrates, including organic electronics (OLED, OPV), sensors, and surface-supported fabrication of graphene. It is, therefore, crucial to study the nature of such interactions on model systems to unravel general trends.

Using a fully non-local vdW density functional (vdW-DF) [1,2] we have studied the adsorption of halogenated benzene, which are simple prototypes for larger and more complex molecules, on stepped and flat Au and Pt surfaces. The effects of various parameters, such as the size of the precursors and type of halogen atoms, on the adsorption properties have also been investigated. Moreover, the calculated potential energy curves revealing both chemisorbed and physisorbed wells, all of which are separated by activation barriers, will be discussed. Specifically for several different adsorption sites of dichlorobenzene, the energies, and equilibrium geometries have been computed, and electron density analysis has been performed using both conventional generalized gradient approximation (GGA) and vdW-DF [3].

[1] M. Dion et al., Phys. Rev. Lett. 92, 246401 (2004).
[2] A. Gulans et al., Phys. Rev. B 79, 201105 (2009).
[3] R. Peköz et al., J. Phys. Chem. C 116, 20409 (2012).

O 18.12 Mon 18:45 H38

Investigations of PEEB adsorbed on metallic surfaces — •L Lokamani, Cormac Toher, Joerg Meyer, Anja Nickel, Robin Ohmann, Francesca Moresco, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

The electronic and tunable optical properties exihibited by p-phenylene-ethynylenes make them excellent candidates for single molecule electronics. A family of derivatives with different electronic properties can be created by adding various functionalzied side groups, which effect the conductance properties of the phenylene-ethynylene backbone. These derivatives with different electronic properties can be utilized to implement novel logic functions in nano circuits.

Here we present the results of a combined theoretical and experimental investigation of the adsorption characteristics, electronic structure and bonding geometry of single 1,4-bis(phenylethynyl)-2,5bis(ethoxy)benzene (PEEB) molecules on the Au(111) surface. DFT calculations of the DOS and adsorption geometry were found to be in qualitative agreement with low temperature STM images and STS measurements. The strength of the bonding interaction to the substrate was also calculated.

O 19: Plasmonics and Nanooptics II

Time: Monday 16:00–19:00 Location: H31

O 19.1 Mon 16:00 H31

Coherent/decoherent coupling of excitations in molecular-plasmonic heterostructures — •Stephanie Cheylan[1], Hongdan Yan[1], Peter Lemmens[1], Meinhard Schilling[2], Andrey Bakin[3], Johannes Ahrens[4], and Martin Bröring[4] — [1]IPKM, TU-BS, Braunschweig — [2]EMG, TU-BS, Braunschweig — [3]IHT, TU-BS, Braunschweig — [4]IAAC, TU-BS, Braunschweig

We study the coherent coupling between plasmons of Au nanowire arrays and excitons of moleculare components, given by BODIPY and its derivative aza-BODIPY. The exciton energy of these two classes of molecules is tuned to match with different plasmonic modes. Different interactions are investigated depending on the morphology of the nanowire array and the energy of molecular excitons. Work supported by DFG, B-IGSM and NTH School for Contacts in Nanosystems.

O 19.2 Mon 16:15 H31

Hybrid waveguide-particle-plasmon-polaritons enhance transverse magneto-optical Kerr effect — •Lars E. Kreilkamp[1], Vladimir I. Belotelov[2], Ilya A. Akimov[1], Manfred Bayer[1], Thomas Wehlus[3], Bernd Stritzker[3], Jessie Chin[4], Stefanie Neutzner[4], Daniel Dregely[4], and Harald Giessen[4] — [1]Experimental Physics 2, TU Dortmund University, D-44221 Dortmund, Germany — [2]A.M. Prokhorov General Physics Institute, Russian Academy of Sciences, 119992 Moscow, Russia — [3]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [4]4th Physics Institute and Research Center SCoPE, University of Stuttgart, D-70569 Stuttgart, Germany

We demonstrate an enhanced transverse magneto-optical Kerr effect (TMOKE) at the optical resonance of a hybrid plasmonic structure. Polaritons are formed by the interaction of particle plasmons in gold nanowires in combination with a slab waveguide mode of the magneto-optical material bismuth iron garnet. A large TMOKE modulates the intensity of a transmitted beam by 1.5% upon switching the magnetization direction. This enhancement of TMOKE is explained by considering a waveguide-particle-plasmon resonance, which shifts and changes its shape upon magnetization flipping and hence leads to a large transmission contrast, in combination with a simultaneously high transmittance. The experimental results are compared to electromagnetic modelling of transmission and TMOKE spectra based on the Rigorous Coupled-Wave Analysis. The influence of surface roughness on the obtainable figure of merit is discussed.

O 19.3 Mon 16:30 H31

One-dimensional plasmons in arrays of monolayer silver wires on Si(557) — •Ulrich Krieg, Yu Zhang, Christian Brand, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany

An array of metallic stripes of monatomic height and up to 10 atoms wide was prepared on the (111)-oriented mini-terraces of vicinal Si (557) via self assembly. By characterization with spot profile analysis LEED (SPA-LEED), STM and electron energy loss spectroscopy (EELS) with both high energy and momentum resolution, we demonstrate that a quasi one-dimensional system was prepared after adsorption between 0.5 and 1 ML of Ag. Only stripes that show $\sqrt{3}\times\sqrt{3}R30^\circ$ order turn out to be metallic with an almost linear dispersion of the plasmonic losses, in the direction parallel to the steps, while in perpendicular direction the plasmonic losses do not disperse at all. Therefore, the wires within the array seem to be electronically decoupled.

Due to the finite width, however, combined inter-subband-plasmon excitations become visible in the direction normal to the wires. The quantitative simulation is compatible with a wire width of 3.6 nm which agrees well with the width of the (111) terraces.

Interestingly, the electron concentration in the wires and thus the slope of the dispersion can be tuned in a wide range by doping these wires, making the Ag wires quite versatile for 1D conductance of plasmonic excitations.

O 19.4 Mon 16:45 H31

In-situ mode selectivity and control in top-down fabricated optical nano-circuits — •Peter Geisler[1], Gary Razinskas[1], Enno Krauss[1], Xiao-Fei Wu[1], Christian Rewitz[2], Phillip Tuchscherer[2], Sebastian Götz[2], Tobias Brixner[2], and Bert Hecht[1] — [1]Experimentelle Physik 5, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Plasmonic modes supported by noble-metal nanostructures offer strong sub-wavelength confinement and therefore promise the realization of nanometer-scale integrated optical circuits with well-defined functionality. The implementation of optical nanocircuitry requires the possibilities to fabricate arbitrary circuit designs as well as to selectively excite, propagate and re-emit specific eigenmodes within a circuit.

In our work we investigate the fundamental properties of micro-fabricated optical two-wire transmission lines. These structures possess two fundamental propagating modes: one that can be identified as an anti-symmetric mode with a field concentration in the gap and an symmetric mode with a mode pattern similar to the mode of a single wire. By carefully optimizing an incoupling antenna and by using well defined illumination conditions it is possible to selectively excite either of both modes. The selective detection of either mode can be achieved by spatially separating the emission spots within a unique mode-detector structure.

O 19.5 Mon 17:00 H31

Coherent control of plasmon propagation in top-down fabricated optical nano-circuits — •Monika Pawłowska[1], Christian Rewitz[1], Sebastian Goetz[1], Peter Geisler[2], Gary Razinskas[2], Enno Krauss[2], Bert Hecht[2,3], and Tobias Brixner[1,3] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Nano-Optics and Biophotonics Group, Experimentelle Physik 5, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Röntgen Center for Complex Material Systems (RCCM), Am Hubland, 97074 Würzburg, Germany

Plasmonic modes supported by noble-metal nanostructures offer strong subwavelength confinement and promise the realization of nanometer-scale integrated optical circuits with well-defined functionality. The coherent control of spatial and temporal energy distribution within a nanostructure is also of high interest. Here, we present the experimental realization of such a coherent control scheme exploiting the interaction of two plasmonic modes propagating on a single gold nanostructure. The structure consists of an input antenna attached to a two-wire transmission line that splits into two branches. It was optimized by finite-difference frequency-domain (FDFD) simulations and fabricated by focused ion-beam milling (FIB). Upon illumination of the antenna with two perpendicularly polarized ultrashort laser pulses two modes can be launched. Since the interference of both modes determines the near-field intensity distribution, the plasmonic energy can be guided towards either arm by controlling the relative phase between the two laser pulses.

O 19.6 Mon 17:15 H31

Large-area 3D chiral plasmonic nanostructures fabricated by colloidal hole mask nanolithography — •Bettina Frank, Jun Zhao, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

We fabricate large-area (square centimeter size) 3D chiral plasmonic nanostructures using colloidal hole mask lithography [1]. We rotate the sample in a polar direction and change the speed of the rotation. Hence, the evaporated amount of metal through the gold holes changes as a function of polar angle. This leads to ramp-like structures and yields true 3D chirality. Additionally, we fabricate a 3D chiral ramp of MgF2 and evaporate a flat strip of gold on top of it. By changing the polar rotation direction, left- as well as right-handed enantiomers can be manufactured. Measuring the transmittance upon circularly polarized light and applying the rules of Hentschel et al. to determine circular dichroism if the sample does not exhibit C3 or C4 symmetry [2], we find a strong chiral optical response with several resonances in the near-infrared between 1 and 3 micrometer wavelength. We are able to interpret this response with the aid of the fundamental modes of the split-ring resonators. Our structures will be very useful for large-area thin-film chiroptical elements and for plasmonic chiral enantiomer sensors.

[1] S. Cataldo et al., ACS Nano 6, 979 (2012).
[2] M. Hentschel et al., Nano Lett 12, 2542 (2012), supplement.

O 19.7 Mon 17:30 H31

Chiral Plasmonic Realization of the Born-Kuhn Model — •Xinghui Yin, Martin Schäferling, and Harald Giessen — 4th Physics Institut, Research Center SCoPE, and Research Center SimTech, University of Stuttgart, Stuttgart, Germany

In recent years, chiral assemblies of plasmonic nanostructures and their associated optical spectra have gained considerable interest [1]. This is due to their ability to generate optical rotatory dispersion (ORD) and circular dichroism (CD) that is orders of magnitude larger than for any naturally occurring substance. Drawing inspiration from the classical theories of optical activity, we investigate a plasmonic version of the most basic system exhibiting chiroptical responses: two coupled anisotropic oscillators that are vertically displaced with respect to each other, known as the Born-Kuhn model [2,3]. It was originally developed to describe two-chromophore coupling in optically active molecules, where each chromophore by itself is achiral. We experimentally realize the Born-Kuhn model of chiral media in a plasmonic system of corner-stacked nanorods and discuss the arising spectra in terms of hybridized modes and retardation effects.

[1] A. Kuzyk et al., Nature **483**, 311 (2012).
[2] M. Born, Z. Phys. A - Hadron Nucl. **16**, 251 (1922).
[3] W. Kuhn, T. Faraday Soc. **26**, 293 (1930).

O 19.8 Mon 17:45 H31

Chiral Fields in Achiral Systems — •Martin Schäferling, Xinghui Yin, and Harald Giessen — 4th Physics Institut, Research Center SCoPE, and Research Center SimTech, University of Stuttgart, Stuttgart, Germany

Chirality – the absence of mirror symmetry – is an integral component of our world. The so-called optical chirality quantifies the chirality of electromagnetic fields [1]. It has been shown that fields with high optical chirality can arise near plasmonic nanostructures with strong planar or three-dimensional geometrical chirality [2].

We demonstrate numerically that geometrical chirality is not a necessary prerequisite for obtaining chiral near-fields: Even a higly symmetric linear plasmonic rod antenna illuminated with linearly polarized light under normal incidence generates chiral electromagnetic fields [3]. We explain this behavior qualitatively by analyzing a Hertzian dipole driven at resonance. This simple model is further utilized to analyze and compare different incident polarizations. We show that the chiral near-field patterns generated by circularly polarized light are still dominated by the distribution found for the linear polarization.

The handedness of the chiral fields near a square structure can be flipped locally by changing the polarization angle of the incident light. Based on these findings, we propose a novel method for enantiomer sensing using linearly polarized light.

[1] Y. Tang and A. E. Cohen, Science **332**, 333 (2011).
[2] M. Schäferling et al., Phys. Rev. X **2**, 031010 (2012).
[3] M. Schäferling et al., Opt. Expr. **20**, 26326 (2012).

O 19.9 Mon 18:00 H31

Adiabatic Nanofocusing on Ultrasmooth Single-Crystalline Gold Tapers Creates a 10-nm-Sized Light Source with Few-Cycle Time Resolution — •Slawa Schmidt[1], Björn Piglosiewicz[1], Diyar Sadiq[1], Javid Shirdel[1], Jae Sung Lee[2], Parinda Vasa[1], Namkyoo Park[2], Dai-Sik Kim[3], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität, Oldenburg — [2]Photonic Systems Laboratory, School of EECS, Seoul National University, Korea — [3]Department of Physics and Astronomy, Seoul National University, Seoul, Korea

We demonstrate adiabatic nanofocusing of few-cycle light pulses using ultrasharp and ultrasmooth single-crystalline gold tapers. We show that the grating-induced launching of spectrally broad-band surface plasmon polariton wavepackets onto the shaft of such a taper generates isolated, point-like light spots with 10 fs duration and 10 nm diameter spatial extent at its very apex. This nanofocusing is so efficient that nanolocalized electric fields inducing strong optical nonlinearities at the tip end are reached with conventional high repetition rate laser oscillators. We use here the resulting second harmonic to fully characterize the time structure of the localized electric field in frequency-resolved interferometric autocorrelation measurements. Our results strongly suggest that these nanometer-sized ultrafast light spots will enable new experiments probing the dynamics of optical excitations of individual metallic, semiconducting, and magnetic nanostructures.

O 19.10 Mon 18:15 H31

Adiabatic nanofocusing of few-cycle laser pulses with wave-front shaping using a deformable mirror — •Pascal Engelke, Slawa Schmidt, Petra Gross, and Christoph Lienau — Institut für Physik, Carl von Ossietzky Universität, Oldenburg, Germany

Adiabatic nanofocusing of ultrashort laser pulses can be used to generate a highly confined light source with few nanometer spatial and few femtoseconds time resolution [1,2]. By grating-coupling a spectrally broad-band light source onto ultra smooth single-crystalline gold tapers, typically coupling efficiencies below 1% are reached. We have identified a wave-front mismatch between the illuminating laser pulses and the conical surface of the tip as a possible cause for the restricted coupling efficiency. Here we demonstrate shaping of the wave front to match the surface radius of curvature using a deformable mirror. The wave front curvature was adapted to the tip surface using an evolutionary algorithm. We found that the coupling efficiency of the light to surface plasmon polariton (SPP) wavepackets was improved considerably, resulting in an enhancement by a factor 8 of the light scattered from the tip apex. Interferometric frequency resolved autocorrelation techniques confirmed that the time structure of the 6-fs pulses was preserved. We anticipate that the demonstrated technique offers considerable improvement for scanning near field optical microscopy techniques.

[1] Berweger, S. et al. Nano Lett. 2011, 11, 4309*4313.
[2] Schmidt, S. et al. ACS Nano 2012, 6, 6040*6048

O 19.11 Mon 18:30 H31

Plasmonic Diastereomers: Adding Up Chiral Centers — •Mario Hentschel[1,2], Martin Schäferling[1], Bernd Metzger[1], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart — [2]Max Planck Institite for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart

We construct chiral plasmonic molecules by assembling two individual chiral centers. Interestingly, depending on the exact arrangement of the centers, all combinations result in a chiral compound with a strong chiral optical response. Furthermore, we demonstrate that the overall circular dichrosim (CD) is determined by the response of the individual chiral centers. We find that the CD spectra of the composite molecules are then simply given as the sum of the CD spectra of the constituting building blocks. Interestingly, as soon as strong near-field coupling takes place between chiral centers, we find strong deviation from the simple additive chiral behavior. Most importantly, we demonstrate that the optical response of complex chiral plasmonic systems [1] can be decomposed and understood in terms of fundamental building blocks, offering simple and straightforward design rules for future applications such as chiral optical elements and enantiomer sensors.

[1] M. Hentschel et al., Nano Lett. 12, 2542 (2012)

O 19.12 Mon 18:45 H31

Nonreciprocal Plasmonics: Thin Film Faraday Rotator — •Jessie Chin[1], Tobias Steinle[1], Thomas Wehlus[2], Thomas Weiss[1], Daniel Dregely[1], Vladimir Belotelov[3], Bernd Stritzker[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCOPE, University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [3]Lomonosov Moscow State University, Faculty of Physics, 119991 Moscow, Russia

Light propagation is usually reciprocal. However, a static magnetic field along the propagation direction can break the time-reversal symmetry in the presence of magneto-optical (MO) materials. The Faraday effect in this material rotates the polarization plane of light, and when light travels backward the polarization is further rotated. It is an important MO effect due to its crucial application in optical isolation. Thin film optical isolators and the enhancement of the MO Faraday effect are of particular interest due to the demand in integrated optics. We report large enhancement of thin film Faraday rotation by a sophisticated plasmonic system hybridized with nonreciprocal MO materials. We present experimental enhancement of Faraday rotation up to one order of magnitude by plasmonics. The enhanced Faraday rotation is accompanied by high transparency, which is favorable for potential applications. Numerical simulations agree very well with the measurement results and explain the mechanism of the enhancement. Our magneto-plasmonic system can be further engineered and may lead to ultracompact device applications in optical systems.

O 20: Surface Chemical Reactions and Heterogeneous Catalysis II

Time: Monday 16:00–19:00 Location: H33

O 20.1 Mon 16:00 H33

Charge Flow and Catalysis at the Metal-Support Interface: The Molecular Nature of Acid-Base Catalysis on Surfaces — •Robert Baker and Gabor Somorjai — University of California, Berkeley - Berkeley, CA, USA

The role of charge transfer to control the activity and selectivity of supported metal catalysts is studied at a molecular level by a range of techniques. Using a platinum/n-type silicon charge-based device, external control of surface oxygen activity is demonstrated using both an electrical bias and a photo-induced current flow. This allows the rate of carbon monoxide oxidation on platinum to be controlled nonthermally with an external bias or with visible light. Analogously, electronic control of surface chemistry is also achieved by substrate doping. Highly n-type, fluorine-doped titanium oxide behaves as an electronically active support for platinum catalysts improving both the rate and selectivity of carbon monoxide oxidation and methanol oxidation by charge transfer to surface oxygen. Finally, sum frequency generation vibrational spectroscopy is used to directly monitor reaction intermediates on supported platinum catalysts. The results show that charge transfer from a titanium oxide support selectively enhances the rate of aldehyde hydrogenation to alcohols by a charge transfer mechanism. These combined studies reveal at a molecular level how charge flow in supported metal catalysts controls surface reaction kinetics and this represents the molecular foundation of heterogeneous acid-base catalysis.

O 20.2 Mon 16:15 H33

CO_2 Capture by Liquid Amine Solutions: A DFT-based Evaluation — •Tugba Davran-Candan and Karsten Reuter — TU München, Germany

Removal of CO_2 from exhaust gases by making use of aqueous amine solutions is a most viable technique to reduce CO_2 emissions that are generally believed to be the major cause of global warming. The amine capture molecules bind CO_2 chemically either in the form of stable carbamates or bicarbonates. However, to date there is no clear understanding of how the specific amine structure favors either of the two binding modes and how it relates to the bond strength. To this end, we perform systematic density-functional theory (DFT) calculations and evaluate the product stabilities (carbamate or bicarbonate) for a wide range of amine molecules. As a reference we compare to the widely investigated monoethanolamine (MEA), where a too high carbamate stability leads to unfavorably high regeneration costs.

O 20.3 Mon 16:30 H33

Bistability during CO oxidation at Pd(100): Atomistic origin from first-principles kinetic Monte Carlo simulations — •Max Hoffmann[1], Matthias Scheffler[2], and Karsten Reuter[1] — [1]TU München, Germany — [2]Fritz-Haber-Institut, Berlin, Germany

Despite numerous studies on Palladium as a catalyst for CO oxidation the nature of the active surface remains debated. Focusing on the (100) surface the pristine metallic surface, an ultra-thin surface oxide, and thicker oxide layers were each suggested as *the* active surface. However, already the fact that the surface state depends sensibly on the reaction conditions challenges the quest to understand the catalytic function in terms of *one* surface state. Hendriksen *et al.* [1] even observed an overlap in stability conditions between a smooth metal surface and a rough oxidic surface state. The two surfaces states were not only found to coexist in different places of the surface, but the entire surface was stabilized in either of the two states at identical reaction conditions.

Using first-principles kinetic Monte Carlo models for the pristine Pd(100) surface and the PdO(101) surface oxide we can reproduce this bistability behavior and furthermore elucidate its atomistic origin. The predicted bistable regime spans stoichiometric and technological reaction conditions. In fact, within this range we find that both surface states exhibit very similar intrinsic reactivity, which puts further doubts on attempts to assign the catalytic function to one *active* state.

[1] B.L.M. Hendriksen, S.C. Bobaru, and J.W.M. Frenken, *Catalysis Today* 105, 234 (2005).

O 20.4 Mon 16:45 H33

Sabatier based Methanation of carbon dioxide and Catalyst stability against contaminations — •Fabian Rachow, Klaus Müller, and Dieter Schmeisser — Brandenburg University of Technology, Applied Physics and Sensors, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

The Sabatier-Reaction $[CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O]$ represents a possible way for the reduction and utilization of CO_2 produced in the oxy-fuel combustion process. While using different ruthenium and nickel based catalysts we studied the catalytic performance with quadrupole mass spectroscopy and IR-spectroscopy in terms of conversion of CO_2, yield of CH_4, selectivity and stability. Conversions of up to 90% and a selectivity of well above 95% could be achieved. Further studies focus on the long term stability, especially with the influence of contaminations like SO_x and NO_x as they may occur in oxy-fuel or flue gas and could greatly reduce the life time of a catalyst. We investigate the limits of Ni based catalysts for those additives. However, technical oxy-fuel gas seems to have no particular effect on the activity of a commonly used NiO-catalyst when compared to quasi pure CO_2, showing only a small drop of performance after five days with a constant conversion rate of over 80% at the end.

O 20.5 Mon 17:00 H33

Reaction kinetics of the Sabatier Reaction in a demonstration plant — •Johannes Israel, Klaus Müller, Fabian Rachow, Guido Beuckert, and Dieter Schmeisser — Technische Universität Cottbus, Applied Physics / Sensor Technologie, Germany

We currently build up a demonstration plant for the direct catalytic conversion of CO_2 into methane according to the Sabatier reaction $CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$.

We have already reached conversion rates higher than 90% and a selectivity close to unity in our laboratory experiments with NiO based catalysts. A good long term stability was obtained with a reactant gas flow density of $0.8l/min \cdot cm^2$ at $350^\circ C$.

We will study the process now on a larger scale with a factor 10000. The process is controlled via mass flow controllers with a throughput of $20m^3/h\ H_2$ and $5m^3/h\ CO_2$ at an inlet gas pressure of up to $15bar$, the temperature is regulated by a PID multichannel controller. As water is a by-product we use an efficient cooling trap for its separation form the obtained methane. The reaction products are analyzed by a quadrupole mass spectrometer under reaction conditions.

We start our experiments in using clean CO_2 and H_2. Later experiments will involve industrial quality (oxy-fuel) conditions also. Goal of this project is to determine the performance of the catalytic process under conditions which enable an industrial implementation in energy storage concepts. In this contribution we report of the design of a demonstration plant and on first experiments concerning the kinetics within the system.

O 20.6 Mon 17:15 H33

Mass transfer effects during near-ambient CO oxidation at Pd(100) in non-ideal reactor chambers — •Sebastian Matera, Max J. Hoffmann, and Karsten Reuter — TU München

A central goal in in-situ studies of defined model catalysts has been to obtain (at best) as resolved spectro- or microscopic information as has been established in UHV surface science. With this focus possible heat and mass transport limitations in the ambient environments have not received much attention. In parts they are even unavoidable, considering the often significant constraints that in-situ techniques impose on the design of the reactor chamber. We investigate such effects with our newly developed first-principles based multi-scale modeling approach integrating kinetic Monte Carlo simulations into a fluid dynamical treatment [1]. Apart from the conceptual discussion in idealized reactor geometries [2], it is in particular the recent integration of our scheme into the general purpose CatalyticFOAM solver [3] that now enables us to also explicitly address the complex flow profiles in actual in-situ reactor chambers. We demonstrate the crucial role of heat and mass transfer limitations, in particular for the unselective and therefore high turnover CO oxidation in the context of recent in-situ XPS and Planar Laser Induced Fluorescence (PLIF) measurements over Pd(100) [4]. [1] S. Matera and K. Reuter, Catal. Lett. 133, 156 (2009). [2] S. Matera and K. Reuter, Phys. Rev. B 82, 085446 (2010); J. Catal. 295,261 (2012). [3] M. Maestri and A. Cuoci, CatalyticFOAM, www.catalyticfoam.polimi.it [4] S. Blomberg, J. Gustafson, E. Lundgren et al., in preparation.

O 20.7 Mon 17:30 H33

Addressing structural and catalytic properties of bimetallic surface alloys using kinetic Monte Carlo — •Luis Mancera and Axel Gross — Institute of Theoretical Chemistry, University of Ulm, D-89069 Ulm, Germany

Using CO as a probe of the local reactivity, it has been experimentally shown that catalytic activity in PdAg/Pd(111) bimetallic surface alloys is mainly driven by the configuration of Pd adsorption sites.[1] Based on density functional theory (DFT) calculations, these ensemble effects have been theoretically confirmed for the same surface alloy, whereas a mutual cancellation of ligand and strain effects has been obtained from the analysis of local density of *d*-states.[2] Since an unexpected dependence of the local reactivity and the formation enthalpy on the subsurface layers has been also found from the DFT calculations, in particular for the case of low silver concentrations at the surface combined with complete silver layers at the subsurface, we address here the effect of diffusion of silver atoms to the sublayers. In order to obtain a more detailed understanding of the catalytic properties by including a wider set of structural configurations, we present in this contribution first steps towards DFT-based kinetic Monte Carlo calculations of bimetallic surface alloys, using PdAg/Pd(111) as a model system.

[1] Y. Ma *et al.* Phys. Chem. Chem. Phys. **13**, 10741 (2011)

[2] L. A. Mancera *et al.* Phys. Chem. Chem. Phys., accepted for publ., DOI:10.1039/C2CP42914D, (2012)

O 20.8 Mon 17:45 H33

Structure and methanol oxidation reaction on $VO_x/TiO_2(110)$ model systems — •Luca Artiglia[1], Stefano Agnoli[1], Andrea Vittadini[2], Alberto Verdini[3], Albano Cossaro[3], Luca Floreano[3], and Gaetano Granozzi[1] — [1]Department of Chemical Sciences, University of Padova, Via Marzolo 1, I-35131, Padova, Italy — [2]ISTM-CNR, Padova, Italy/PD I-35131, Italy — [3]TASC National Laboratory, CNR-IOM, Trieste, Italy/TS I-34149, Italy

During the past years the structure of vanadia (VO_x) thin films supported on TiO_2 rutile (110) and their reactivity towards alcohols oxidation have been extensively studied. The main reaction products are aldehydes, thus the reaction proceeds through oxidative dehydrogenation (ODH) path. In this work we introduce a completely new set of data collected on different amount of VO_x (from 0.2 to 2.0 ML) grown on TiO_2 (110) by V reactive deposition in O_2, where the V oxidation state is close to +4. A complete surface science characterization (XPS, XPD and STM) and DFT calculations have allowed us to describe the structure and electronic properties of VO_x nanoclusters (NCs), obtained after 0.2 ML V deposition. These NCs resulted to be V_4O_8 tetramers growing aligned along the TiO_2 [001] crystallographic direction. Hence we have focused on the interaction between VO_x/TiO_2 model system and methanol performing TPD experiments. Our results clearly show that on VO_x tetramers ODH reaction takes place at low temperature (ca. 290 K) and that the system selectivity is high. A TPD analysis of higher VO_x coverage (up to 2.0 ML) unravel a desorption peak shift to lower temperatures together with a selectivity decrease.

O 20.9 Mon 18:00 H33

Methanol synthesis on ZnO from molecular dynamics — •Johannes Frenzel and Dominik Marx — LS Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

Advanced molecular dynamics [1] is demonstrated to be a powerful, comprehensive and general approach to study surface chemical reactions using such as those underlying the heterogeneous catalytic synthesis of methanol from CO on ZnO as a case study[2,3]. This technique opens up a novel dimension in moving closer to the experiment by allowing to explore enormous space of chemical possibilities generating an unexpectedly complex reaction network of apparently simple surface chemical reactions in the first place. In particular, "near-surface states" are identified to be key to some of the steps in the catalytic cycle tanking place at ZnO($000\bar{1}$) surface with oxygen vacancies[4].

Automated exploration techniques in the framework of accelerated molecular dynamics, as opposed to genuinely static approaches, might be the method of choice to address such problems involving competing processes to the molecule-surface interaction.

[1] A. Laio and M. Parrinello, *PNAS* **99** (2002) 12562; M. Iannuzzi, A. Laio and M. Parrinello, *Phys. Rev. Lett.* **90** (2003) 238302

[2] J. Kiss, J. Frenzel, N. N. Nair, B. Meyer and D. Marx, JCP **90** (2011) 064710

[3] J. Frenzel, J. Kiss, N. N. Nair, B. Meyer and D. Marx, submitted

[4] J. Kiss, A. Witt, B. Meyer and D. Marx, JPC **130** (2009) 184706

O 20.10 Mon 18:15 H33

Flow-Reactor Investigations of Clean and Cs-promoted Ag foils as Catalysts in the Ethylene Epoxidation Reaction — Gergely Rozsa, •Regina Wyrwich, Sebastian Böcklein, Maximilian Ganiek, and Joost Wintterlin — Department Chemie, Ludwig-Maximilians-Universität München, Germany

The selective epoxidation of ethylene over Ag is a large scale industrial process. Nevertheless the reaction mechanism is still heavily debated. In the commercial process a supported catalyst is used and Cs is added as a promotor to improve the selectivity. Despite intense investigations on model systems the role of Cs remains unclear. Both a site blocking effect as well as an electronic effect are discussed. In the context of an extensive catalytic study we investigated the behaviour of Cs-promoted polycrystalline Ag-foils under reaction conditions. We report about a procedure to reproducibly deposit Cs on sputter-cleaned Ag foils by dip-coating in aqueous CsOH solutions. Based on x-ray photoelectron spectroscopy (XPS) measurements a Langmuir-type behaviour of the deposition process is observed. Evaluation and comparison of the catalytic performance (activity and selectivity) of the Cs-promoted and clean Ag foils is done in a flow-reactor setup with quadrupole mass spectrometry (QMS) for product analysis. A crucial dependency upon the activation procedure (thermal treatment at 500 °C in Ar or O_2) is found in this case. A potential influence of Cs seems to arise at higher pressures of the reactant gases indicating a site blocking effect of Cs.

O 20.11 Mon 18:30 H33

Ethylene Oxide Formation over Ag(111): Reactivity and Spectroscopy Investigation of the Active Oxygen Species

— •Sebastian Böcklein[1], Sebastian Günther[2], and Joost Wintterlin[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Technische Universität München, Germany

Despite intensive investigation the ethylene oxide (EtO) formation over Ag catalysts remains an unsolved problem. By applying a special preparation procedure we were able to obtain and characterize the catalytically active oxygen phase on Ag(111). Reactivity experiments of this species with ethylene using temperature-programmed reaction (TPR) show formation of EtO. X-ray photoelectron spectroscopy (XPS) gives an O 1s signal in the range of 530-531 eV. A closer investigation of the XPS data shows that it consists of two distinct oxygen species (O 1s BE 530.2 and 530.7 eV). The ratio depends on the simulataneous presence of the p(4×4)O reconstruction and on the sample temperature. Temperature dependent XPS (TDXPS) measurements show that the 530.2 eV-species increases with temperature, and a quantitative analysis indicates a reversible transformation between the two species. By angle resolved XPS (ARXPS) depth profiles for these species could be evaluated resulting in a model for this system. Using in situ scanning tunneling microscopy (STM) we could follow the reaction of this reactive oxygen phase with ethylene. The reaction is connected with massive changes of the catalyst surface and with the appearance of new ordered structures like a (2×2) or a chain-like phase.

O 20.12 Mon 18:45 H33

Bonding of ammonia and its dehydrogenated fragments on Ru(0001) — •Sabine Maier[1], Ingeborg Stass[2], Jorge Cerda[3], and Miquel Salmeron[4] — [1]University of Erlangen-Nürnberg, Department of Physics, Erlangen, Germany — [2]Freie Universität Berlin, Institut für Experimental Physik, Berlin, Germany — [3]CSIC, Instituto de Ciencia de Materiales, Madrid, Spain — [4]Lawrence Berkeley National Laboratory, Materials Science, Berkeley, CA, United States

The catalytic ammonia decomposition has recently attracted attention due to the high hydrogen storage capacity of ammonia and the possibility to produce hydrogen without toxic or greenhouse gases as byproducts, making ammonia a potential candidate as an energy carrier for fuel cells. Here we present low temperature scanning tunneling microscopy experiments and density functional theory calculations that unambiguously establish the adsorption sites of the NH_x (x=0-3) species and give insights into the dissociation pathways of ammonia on Ru(0001). All the N-H bond cleavage reactions were induced by controlled tip manipulation to produce each of the NH_x (x=0-2) intermediates. Further, the interaction of ammonia with surface hydrogen and the ammonia dimer formation will be discussed.

O 21: Electronic Structure and Spin-Orbit Interaction I

Time: Monday 16:00–18:45 Location: H42

O 21.1 Mon 16:00 H42

A non-local density functional by explicitly modeling of the exchange-correlation hole in inhomogeneous systems — •Klaas J.H. Giesbertz[1], Robert van Leeuwen[2], and Ulf von Barth[3] — [1]Department of Theoretical Chemistry, Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands — [2]Department of Physics, Nanoscience Center, University of Jyväskylä, P.O. Box 35, 40014 Jyväskylä, Survontie 9, Jyväskylä, Finland — [3]Department of Mathematical Physics, Institute of Physics, Lund University, Sölvegatan 14A, Lund S-22362, Sweden

We develop a non-local density functional by a direct modeling of the shape of exchange-correlation (xc) hole in inhomogeneous systems. The functional is aimed at giving an accurate xc-energy and an accurate corresponding xc-potential even in difficult near-degeneracy situations such as molecular bond breaking. In particular we demand that: (1) the xc hole properly contains -1 electron, (2) the xc-potential has the asymptotic $-1/r$ behavior outside finite systems and (3) the xc-potential has the correct step structure related to the derivative discontinuities of the xc-energy functional. These demands are achieved by screening the exchange hole in such a way that the pair-correlation function is symmetric and satisfies the sum-rule. These two features immediately imply (1) and (2) while the explicit dependence of the exchange hole on the Kohn–Sham orbitals implies (3). For the dissociating hydrogen molecule, we obtain much improved xc holes and thus also improved binding energies at different interatomic distances, as compared to the local density approximation.

O 21.2 Mon 16:15 H42

Description of Rabi oscillations within time-dependent density functional theory — •Jeiran Jokar and Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Many physical processes stemming from the interaction of light with matter are non-linear in nature. A prototype of such a process is the Rabi oscillation, i.e. the oscillation between the ground state and an excited state when a monochromatic laser with a frequency close to the resonance is applied. It is one of the few analytically solvable cases of non-linear electron dynamics where the population of states changes dramatically in time. Due to the resulting change in the density the description of Rabi oscillations by density functional theory (DFT) suffers from shortcomings that can be traced back to the use of adiabatic approximations which leads to a time-dependent detuning of the resonant frequency. Here, we investigate Rabi oscillations in a one-dimensional model system containing two electrons in a triplet configuration using exact exchange (EXX) and the adiabatic local density approximation (ALDA) within time-dependent DFT. Contrary to the singlet case, where no resonant Rabi oscillations can be observed, we find that the EXX and ALDA calculations for the triplet state show a near-resonant behavior. A small detuning of the laser frequency even results in a resonant Rabi oscillation in the EXX case which hints at the detuning due to the approximate functional being constant in time. We discuss the differences between the singlet and the triplet excitations which lead to a time-dependent or constant detuning, respectively.

O 21.3 Mon 16:30 H42

Double excitations from modified Hartree-Fock equations — •Iris Theophilou[1], Maria Tassi[2], and Stavros Thanos[2] — [1]Peter Grünberg Institut (PGI) and Institute for Advanced Simulation (IAS) Forschungszentrum Jülich D-52425 Jülich, Germany — [2]Institute of Material Science, National Center for Scientific Research Demokritos, 15310, Athens, Greece

While doubly excited states have become important in technological applications, e.g. in increasing the efficiency of solar cells, their description using ab initio methods is a great theoretical challenge because double excitations cannot be described in linear response based on a single Slater determinant. We recently developed a modified Hartree-Fock (HF) approximation for calculating singly excited states [1]. In the present work we extend this method further to also allow for the description of doubly excited states. We describe the double excitation as two holes in the subspace spanned from the occupied HF orbitals and two particles in the subspace of virtual HF orbitals. A subsequent minimization of the energy optimizes the representation of both the holes and the particles in the occupied and virtual subspaces, respectively. We test our method for various atoms and polyene molecules which are known to have excitations with significant double excitation character.

[1] M.Tassi., I.Theophilou, and S.Thanos, Int. J. Quantum Chem. 2012 DOI:10.1002/qua.24049

O 21.4 Mon 16:45 H42

Accurate calculation of optical excitations for large systems — •Margherita Marsili[1] and Paolo Umari[1,2] — [1]Dipartimento di Fisica e Astronomia, Universitá di Padova, via Marzolo 8, I-35131 Padova, Italy — [2]CNR-IOM, Theory@Elettra group, Trieste, Italy

Many-body perturbation theory is the natural framework for the description of electronic excited state properties. For instance, within MBPT, single-particle excitation energies (as probed by photoemission and STS experiments) are found at the poles of the single particle Green's function. Response functions, describing optical spectra, are calculated via the solution of the Bethe-Salpeter equation (BSE), which explicitly contains the electron-hole interaction.When excitonic effects are neglected, absorption spectra are often in bad agreement with the experiments. The agreement with experiment is restored when the electron-hole interactions are included. Excited states are in this case described as linear combinations of independent-particle transition. Although very accurate, the appealing of the BSE scheme is limited due to its high computational cost. We will show how we can enlarge the scope of BSE calculations. First, we the use maximally localized Wannier's functions for reducing strongly the terms which need to to be calculated for evaluating the electron-hole interaction Then, we avoid any explicit sum over empty one-particle orbitals. As a consequence we are able to determine, not only the excitation spectra, but also, directly, each excited state. We validate our scheme by addressing the optical excitations of small isolated molecules. Finally, we will illustrate a few examples where larger systems are investigated.

O 21.5 Mon 17:00 H42

Frequency-dependent electron-hole interaction in the calculation of absorption spectra — •Lorenzo Sponza[1,2], Matteo Guzzo[1,2], Christine Giorgetti[1,2], and Lucia Reining[1,2] — [1]LSI - Ecole Polytechnique — [2]European Theoretical Spectroscopy Facility

State of the art calculations of optical spectra rely on the Bethe-Salpeter Equation (BSE) which is usually solved in a static approximation. The inclusion of dynamical effects is however crucial to describe aspects important e.g. in the design of some high efficiency solar devices[1]. Even if different attempts to perform dynamical-BSE exist[2,3,4], there is still the need for a more efficient and flexible method that would allow one to cover all aspects for realistic systems.

We devised a two step scheme to include dynamical effects in optical spectra. To this aim, we first evaluate dynamical effects in the independent e-h correlation function as a pre-processing method that relies on the solution of an integro-differential equation[5]. Then, using this result as input for an appropriate static BSE-like equation, we evaluate the full spectra including dynamical effects. Our results explains when those effects are strong, and when they are instead weakened by interference effects.

[1] For a review see A.J.Nozik, Chem.Phys.Lett **457**, 3 (2008)

[2] F.Bechsted et al, Phys.Rev.Lett. **78**, 1528 (1997)

[3] D.Sangalli et al, J.Chem.Phys **134**, 034115 (2011)

[4] A.Marini and R.Del Sole, Phys.Rev.Lett. **91**, 176402-1 (2003)

[5] See also: G.Lani, P.Romaniello, L.Reining New J.Phys. **14**, 013056 (2012) and M. Guzzo et al. Phys.Rev.Lett. **107**, 166401 (2011)

O 21.6 Mon 17:15 H42

Spin polarization of (001) surface states of the topological crystalline insulator Pb$_{1-x}$Sn$_x$Se — •Bastian M. Wojek[1], Ryszard Buczko[2], Piotr Dziawa[2], Bogdan J. Kowalski[2], Magnus H. Berntsen[1], Balasubramanian Thiagarajan[3], Andrzej Szczerbakow[2], Perła Kacman[2], Tomasz Story[2], and Oscar Tjernberg[1] — [1]KTH Royal Institute of Technology, Stockholm, Sweden — [2]Institute of Physics, Polish Academy of Sciences, Warsaw, Poland — [3]MAX IV Laboratory, Lund University, Lund, Sweden

It has recently been discovered, that the narrow-gap IV-VI semiconductor Pb$_{1-x}$Sn$_x$Se undergoes a transition from a normal insulator into a topological-crystalline-insulating (TCI) state when the band structure is inverted at large enough Sn content and low temperatures [P. Dziawa *et al.*, Nat. Mater. **11**, 1023–1027 (2012)]. In the TCI phase, the mirror symmetry of the crystal warrants the topological protection of metallic surface states in this material [T. H. Hsieh *et al.*, Nat. Commun. **3**, 982 (2012)].

Here, we study the (001) surface states of Pb$_{1-x}$Sn$_x$Se. Our calculations not only predict metallic surface states with a chiral spin structure for the TCI state but also gapped surface states with nonzero polarization when the system is a normal insulator. For both phases, angle- and spin-resolved photoemission experiments provide conclusive evidence for the formation of these surface states and their chiral spin structure.

O 21.7 Mon 17:30 H42

Spin texture and circular dichroism in photoelectron spectroscopy from the topological insulator Bi$_2$Te$_3$: First-principles photoemission calculations — •Hossein Mirhosseini[1] and Jürgen Henk[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

By relativistic first-principles photoemission calculations for the topological insulator Bi$_2$Te$_3$, we study how the spin texture of the Dirac state manifests itself in circular dichroism [1]. On one hand, there are significant modifications of the initial state's spin texture, which are explained by final-state effects and the symmetry of the photoemission set-up. On the other hand, a highly symmetric set-up allows to conclude on the detailed Dirac state's spin texture. Our study supports that circular dichroism in angular distribution successfully complements spin- and angle-resolved photoelectron spectroscopy from topological insulators.

[1] H. Mirhosseini and J. Henk, Phys. Rev. Lett. **109** (2012) 036803.

O 21.8 Mon 17:45 H42

Electronic structure and photoemission of topological insulators — •Jürgen Braun, Jan Minar, and Hubert Ebert — Dept. Chemie und Biochemie, LMU Universität München, Germany

We discuss calculated spectral features of Bi$_2$Te$_3$, Bi$_2$Se$_3$ and Sb$_2$Te$_3$ and compare with corresponding experimental data. In detail, the dependence of the CDAD on the photon energy is identified as a final state effect. Furthermore, a complete calculation of the spin-polarization vector including the component perpendicular to the surface is presented. Also the behavior of Rashba split surface resonances which had been observed at higher binding energies is analysed. Last but not least the unoccupied bulk and surface states of these materials are investigated by use of our one-step photoemission theory. The calculations have been performed in the framework of the fully relativistic version of the one-step model that is part of the Munich SPR-KKR program package [1]. To guarantee for a quantitative description of the surface-sensitive spectral features special attention is payed to the image-potential behavior of the surface barrier, which is included as an additional layer in the photoemission formalism.

1. H. Ebert et al., The Munich SPR-KKR package, version 6.3, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2012).

O 21.9 Mon 18:00 H42

Spin-dependent unoccupied electronic structure of the topological insulator Bi$_2$Se$_3$: An inverse-photoemission study — •Anna Zumbülte[1], Christian Langenkämper[1], Anke B. Schmidt[1], Markus Donath[1], Tobias Förster[2], Peter Krüger[2], Marco Bianchi[3], Richard Hatch[3], Philip Hofmann[3], Jianli Mi[4], and Bo Brummerstedt Iversen[4] — [1]Physikalisches Institut, Universität Münster — [2]Institut für Festkörpertheorie, Universität Münster — [3]Department of Physics and Astronomy, Aarhus University — [4]Department of Chemistry, Aarhus University

In recent years, topological insulators have become a focus of photoemission studies. Especially the spin-dependent electronic structure shows still surprising features, e.g. the evolution of Rashba-split quantum well states due to a strong surface band bending. With regard to possible devices and the interpretation of non-equilibrium behavior of topological insulators, the additional knowledge of their unoccupied electronic structure is essential.

In this talk, we present spin-resolved inverse-photoemission measurements on a prototypical topological insulator: Bi$_2$Se$_3$. While for higher energies bulk-derived features seem to dominate the obtained data, several features with distinct spin asymmetries are observable at energies up to 2 eV above the Fermi level. The nature of these will be discussed along with theoretical calculations including a long-ranged potential to simulate a band bending. In particular, these calculations predict an unoccupied W-shaped spin-split surface state which we observe experimentally at 1 eV above the Fermi level.

O 21.10 Mon 18:15 H42

Influence of adsorbates on the electronic structure of the topological insulator Bi$_2$Se$_3$: ab-initio investigations — •T. Förster[1], P. Krüger[1], M. Rohlfing[1], A. Zumbülte[2], C. Langenkämper[2], A. B. Schmidt[2], and M. Donath[2] — [1]Institut für Festkörpertheorie, Universität Münster, Germany — [2]Physikalisches Institut, Universität Münster, Germany

Topological insulators possess helical surface states that are protected by time reversal symmetry. Additionally, traditional surface states exist. The rich physics of these systems is determined by the actual boundary conditions at the surface which can distinctly be affected by adatoms. Using density-functional calculations, we investigate the influence of adsorbates on the electronic structure of the Bi$_2$Se$_3$ surface. First, the effect of an adsorbate induced two-dimensional electron gas at the surface is studied by adding a respective long-ranged potential $V(z)$ to the self-consistent one. This simple approach already leads to a down-shift of the Dirac point and the appearance of additional Rashba-like surface states similar to the findings of various experiments. In addition to this, we observe a W-shaped spin-split surface state in the unoccupied part of the band structure. This previously undescribed state is also seen in spin-resolved inverse-photoemission experiments. Secondly, our calculations show that monolayers of hydrogen or potassium adatoms give rise to long-ranged surface potentials and thus also induce the above mentioned features in the band structure. Furthermore, we find surface states that are specific to H and K, respectively.

O 21.11 Mon 18:30 H42

Dirac-cone-like surface state in W(110): Dispersion, spin texture, and photoemission from first principles — Hossein Mirhosseini[1], •Markus Flieger[2], and Jürgen Henk[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

We report on a theoretical study of a d_{z^2} surface state at the tungsten (110) surface, addressing in detail the spin-resolved electronic structure as well as photoemission spectroscopy. In agreement with recent experiments [1], this surface state shows a strongly anisotropic dispersion: In the $\overline{\mathrm{H}}$–$\overline{\Gamma}$–$\overline{\mathrm{H}}$ direction of the surface Brillouin zone, it disperses linearly but becomes flattened along the $\overline{\mathrm{N}}$–$\overline{\Gamma}$–$\overline{\mathrm{N}}$ direction. The *ab initio* calculated spin texture agrees with the one derived from a model Hamiltonian; due to two-fold surface symmetry and time-reversal symmetry, the out-of-plane spin polarization vanishes. The photoemission intensities depend sensitively on the polarization of the incident light, because of the orbital composition of the surface state. The photoelectrons become spin-polarized out-of-plane, which is attributed to breaking the time-reversal symmetry by the excitation process.

[1] K. Miyamoto *et alii*, Phys. Rev. Lett. **108** (2012) 066808; *eidem*, Phys. Rev. B **86** (2012) 161411(R).

O 22: Nanostructures at Surfaces II

Time: Monday 16:00–18:45 Location: H45

O 22.1 Mon 16:00 H45

Self-assembly of Fe cluster superlattice in metal-organic network — Marina Pivetta[1], •Giulia E. Pacchioni[1], Uta Schlickum[1,2], Johannes V. Barth[3], and Harald Brune[1] — [1]Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [2]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [3]Physik Department E20, Technische Universität München, D-85748 Garching, Germany

We studied the self-assembly of Fe clusters and adatoms in a metal-organic honeycomb network on Cu(111) by means of low-temperature scanning tunneling microscopy. The network is formed by coordination of dicarbonitrile pentaphenyl molecules to Cu adatoms. Fe atoms landing on the metal surface are mobile and are steerd by the quantum confinement of the surface state electrons towards the center of the network hexagonal cavities. In cavities with more than one Fe atom, preferential interatomic distances are observed. Upon gentle annealing the adatoms in each hexagon aggregate into a single cluster. These clusters are again centered in the cavities and their size is discerned by their distinct apparent heights.

O 22.2 Mon 16:15 H45

Multipotent mesenchymal stem cells (MSCs) and osteoblasts (OB) on SiO2 nanopillar arrays: Effect of pillar geometry on cell adhesion, proliferation and viability — •Burcin Özdemir[1], Alfred Plettl[1], Jörg Fiedler[2], Jochen Bartholomä[2], Paul Ziemann[1], and Rolf Brenner[2] — [1]Institute of Solid State Physics — [2]Departments of Orthopedics, University of Ulm, Germany

In this contribution, we quantitatively investigate the behavior of MSCs and OB as influenced by systematically nanostructured SiO2 surfaces in order to develop optimized interfacial interactions between cells and substrate for orthopedic device design. Diblock-copolymer micelle nanolithography (BCML) is applied in combination with photochemical growth to obtain highly ordered Au nanoparticles in 2D-arrays, which, subsequently, are used as nanomasks for anisotropic reactive ion etching (RIE). Cyclic combination of photochemical growth and RIE results in well-defined hexagonally ordered SiO2 nanopillar arrays with heights up to 320 nm (maximum aspect ratio ~9:1). Ten different SiO2 nanopillar arrays combining heights of 20 and 50 nm with interpillar distances of 50, 100, 120 nm and diameters of 10, 30 nm were analyzed by high resolution scanning microscopy and immunofluorescence. Highest proliferation rate for MSC was observed on the nanopillar arrays with dimensions of 10-100-50 nm (width, distance, height). Osteogenic differentiation, however, is significantly induced by shorter pillar heights.SEM examination showed that regardless of the 3D structure of the cells, they mainly adhered to the very tops of the pillars.

O 22.3 Mon 16:30 H45

Surface-assisted organic synthesis: Hyper-benzene nanotroughs on Cu(111) — Qitang Fan[1], Cici Wang[1], Yong Han[1], Junfa Zhu[1], Julian Kuttner[2], Gerhard Hilt[2], and •J. Michael Gottfried[2] — [1]National Synchrotron Radiation Laboratory, University of Science and Technology of China — [2]Fachbereich Chemie, Philipps-Universität Marburg

The surface-assisted synthesis of organic nanostructures is a promising bottom-up approach for the functionalization of surfaces in view of applications in catalysis, sensor systems, or organic electronics. The major challenge of this approach is that most established organic reactions require a solvent and thus cannot be performed on "dry" surfaces in UHV. An exception is the Ullmann reaction, which achieves C-C coupling between haloarene molecules by means of metallic Cu and has recently been employed to prepare 1D and 2D polymers on metal single-crystal surfaces. In our combined STM/XPS study, we used specially designed bromo-terphenyl precursors in a UHV-compatible variant of the Ullmann reaction to prepare cyclo-octadeca-phenylene (hyper-benzene), a cyclic hexagonal molecule consisting of 18 phenylene units, on a Cu(111) surface. The molecules arrange in close-packed islands with a hexagonal unit cell. The inner diameter of the hyper-benzene molecules is 2.13 nm, which makes them interesting candidates for nanotroughs that can enclose metal particles or organic molecules. Besides these large hydrocarbon molecules, we will describe the growth of zigzag-shaped 1D organometallic polymers consisting of Cu-bridged oligophenylene units.

O 22.4 Mon 16:45 H45

Stitch-free Electron Beam Lithography of Bragg Gratings and Photonic Crystals — Michael Kahl[1], •Jörg Stodolka[1], and Kevin Burcham[2] — [1]Raith GmbH, Konrad-Adenauer-Allee 8, Dortmund, 44263, Germany — [2]Raith USA, Inc., 2805 Veterans Highway, Suite 23, Ronkonkoma, NY 11779

We report on a new exposure mode for eliminating stitching errors and increasing the throughput in vector scan electron and ion beam lithography (EBL/IBL) of large-area, periodic micro and nano structures. When using the modulated beam moving stage (MBMS) exposure mode, beam movement is controlled in a way that the combination of patterning and continuous movement of a laser interferometer stage results in stitch-free, strip-shaped periodic structures.

The new mode has been used to expose 50 microns wide and 1 mm long gratings with a pitch within a 0.1nm tolerance for the target pitch across the complete grating, demonstrating that MBMS can fabricate periodic structures with virtually no stitching errors in the direction of stage motion. Furthermore, MBMS significantly increases throughput by reducing the times associated with stage motion, pattern data preparation and transfer, and beam settling times. Moreover, 2D arrays of circles or of any other patterns can be written with corresponding complex beam patterns, both as strip-shaped and area structures. The DFB laser gratings and photonic crystals presented in this report are just the first application examples, indicating the potential of MBMS for writing periodic structures for multiple applications such as plasmonic structures in sensors and nano sieves.

O 22.5 Mon 17:00 H45

Highly resolved KPFM investigations on gold and silver nano-dot arrays on silicon — •Anne-D. Müller[1], Yan Mi[2], Kin-Mun Wong[2], Falk Müller[1], and Yong Lei[2] — [1]Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz, Germany — [2]TU Ilmenau, Institute of Physics & INM (ZIK), Threedimensional Nanostructuring, 98684 Ilmenau, Germany

This contibution demonstrates highly resolved Kelvin Probe Force Microscopy (KPFM) results and EFM on ordered gold and silver quantum dot arrays deposited in a template structure on silicon. These quantum dots exhibit a one by one relation between dot spacing and dot diameter and are almost as wide as high. As the quality and quantifiablility of KPFM results usually strongly is influenced by topographical features, the KPFM investigation of such samples usually should not produce reliable results. This contribution demonstrates that due to the usage of specialized cantilevers, KPFM measurements with less than 10 nm resolution are possible on such topographically complicated samples.

O 22.6 Mon 17:15 H45

Self-Doping on Si(111)-(5x2)-Au: Confined Charge Density and Atomic Origin of Electron States — •Ingo Barke, Stefan Polei, Viola v. Oeynhausen, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

Using atomically precise scanning tunneling spectroscopy (STS) the concept of doping is pushed to the ultimate limit. On an array of atomic chains on Si(111)-(5x2)-Au it is shown that single doping atoms contribute their electrons to a small chain section, terminated by the very dopants themselves [1]. Such confined doping is a direct consequence of reduced dimensionality and is not observed in higher dimensions. This contribution focuses on the particular states affected by local doping on Si(111)-(5x2)-Au. Their doping-dependent energy shift and atomic origin is discussed on the basis of high-resolution STS-maps.

[1] I. Barke, S. Polei, V. von Oeynhausen, and K.-H. Meiwes-Broer, Phys. Rev. Lett, **109**, 066801 (2012).

O 22.7 Mon 17:30 H45

Structural Phase Transition on Si(553)-Au: Temperature and Tunneling Current Dependence — •Stefan Polei[1], Ingo Barke[1], Paul Snijders[2], and Karl-Heinz Meiwes-Broer[1] — [1]Institut für Physik, Universität Rostock, Rostock, Germany — [2]Materials Science & Technology Division, Oak Ridge Nat. Lab., Oak Ridge, Tennessee, USA

Atomic chains on semiconductor surfaces have gained considerable interest in the last few years because they are a promising model system for low dimensional physics. On Si(553)-Au earlier studies revealed competing periodicities of 1x2 and 1x3 unit cells [1]. Recently, the frequently observed 1x3 structure was attributed to a spin-polarized ground state with antiferromagnetic ordering [2]. In this contribution we present Scanning Tunneling Microscopy (STM) measurements of the Si(553)-Au surface at various temperatures and tunneling conditions. The periodicity of the Si step-edge chain is found to change gradually from 1x3 to 1x2 depending on temperature and magnitude of the tunneling current. As a consequence, the STM topography shows an apparent 1x6 structure in the transition regime. A Fourier-based analysis of the observed periodicities allows the deduction of a qualitative phase diagram as a function of current and temperature.

[1] P. C. Snijders et al., PRL 96, 076801 (2006); [2] S. C. Erwin, F. J. Himpsel, Nat. Commun. 1, 58 (2010)

O 22.8 Mon 17:45 H45

Optical Anisotropy Spectroscopy of metallic Nanowires on vicinal Semiconductor Surfaces — •Jochen Räthel[1], Eugen Speiser[1], Sebastian Meyer[2], Julian Aulbach[2], Lenart Dudy[2], Jörg Schäfer[2], Daniel Lükermann[3], Ulrich Krieg[3], Christoph Tegenkamp[3], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Albert-Einstein-Str. 9, 12489 Berlin — [2]Universität Würzburg, Physikalisches Institut, Am Hubland, 97074 Würzburg — [3]Institut für Festkörperphysik, Leibniz-Universität Hannover, Appelstraße 2, 30167 Hannover

Metals adsorbed on semiconductor surfaces allow a variety of different surface reconstructions. Among them are one-dimensional structures, often denoted as atomic quantum chains, which preferably grow on vicinal substrates. These chains host exotic electronic ground states, e.g. a charge-density wave state reported for In on Si(111) and Au on Si(553), a insulator-to-metal transition in In on Si(111) and Pb on Si(557) or the rare Tomonaga-Luttinger liquid phase in Au on Ge(001). This talk will briefly introduce these four types of wires from their optical properties as deduced from reflection anisotropy spectroscopy (RAS) of linear polarized light at normal incidence. The response gives access to optical transitions within the band structure from the IR to the UV spectral range. Combined with calculated optical spectra by ab-initio density functional theory the experimental data provide a bases for structural modeling of these complex surface reconstructions [PRL 102, 226805 (2009)].

O 22.9 Mon 18:00 H45

Evolution of microstructure and magnetic properties of amorphous FeNiP nanowire arrays upon annealing — •Nina Winkler, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm Str. 10, 48149 Münster, Germany

Amorphous soft magnetic materials are suitable for application in high frequency, high power conversion and many further research fields. In this work, the fabrication of amorphous FeNiP nanowire arrays with large aspect ratios using porous Anodic Aluminum Oxide (AAO) templates will be presented.

The AAO template exhibits high hexagonal regularity of cylindrical pores which are perpendicularly arranged with respect to the Al substrate plane. The pore diameters used for the fabrication are 20 nm to 250 nm with lengths up to 40 μm. FeNiP nanowire arrays are prepared by filling the AAO pores via electrodeposition using a potential pulse sequence. The electrodeposition parameters are analyzed via cyclic voltammetry. The structure of the nanowire arrays has been characterized by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The magnetic properties of the nanowire arrays have been investigated by Vibrating Sample Magnetometer (VSM) measurements.

Fully amorphous FeNiP nanowires were obtained. Upon in-situ annealing in the TEM, long range diffusion leading to crystallization was observed, which naturally also triggered changes of the magnetic properties.

O 22.10 Mon 18:15 H45

Growth and properties of thin Bismuth films on vicinal Silicon substrates — •Christian Brand, Daniel Lükermann, Saddam Banyoudeh, Dennis Laube, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

The semimetal Bismuth has recently come back into the focus of research due to its particular electronic properties. Low carrier concentrations in combination with small effective masses but high surface conductivity and a large Rashba splitting reveal thin Bismuth films as interesting object. Growth experiments of vicinal Bismuth films, which are expected to reveal topologically non-trivial edge states, were not performed so far. In the present work we studied the growth of ultrathin Bismuth films on vicinal Si(557) substrates by means of *SPA-LEED* and *STM/STS*. (Sub-)Monolayer (ML) thin films as wetting-layer structures with $(\sqrt{3} \times \sqrt{3})$ reconstruction strongly influence the orientation and electronic properties of thicker Bismuth films (40 bilayers) grown on the substrate. Refacetting of the (557) surface occurs at low Bismuth coverages (and high temperatures) introducing (113) and (335) facets on the α-phase (1/3 ML), while (113) and (3 3 10) facets are formed on the so called γ-phase (2/3 ML). Only on the β-phase (1 ML) the initial step structure is preserved. In particular, stepped Bi(110) films with varying, but oriented rotational domains can be grown, while stepped and rotationally disordered Bi(111) films only grow on the α-phase. The steps have been characterized by first DC- and magneto-transport measurements.

O 22.11 Mon 18:30 H45

Investigation of the doping profile of Zn-doped GaAs nanowires by a multitip STM — •Matthias Steidl[1,4], Weihong Zhao[1,4], Werner Prost[2], Stefan Korte[3], Bert Voigtländer[3], Peter Kleinschmidt[5,4], and Thomas Hannappel[1,4,5] — [1]Institut für Physik, Fachgebiet Photovoltaik, TU Ilmenau, D-98684 Ilmenau — [2]Lehrstuhl für Halbleitertechnik/Halbleitertechnologie, Universität Duisburg-Essen, D-47048 Duisburg — [3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, D-52425 Jülich, Germany — [4]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [5]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

III-V semiconductor nanowires (NWs) are promising building blocks for novel semiconductor devices in future electronic and opto-electronic applications such as solar cells. In this context a homogeneous distribution of the dopant over the whole NW is of great importance. We have grown p-type Zn-doped GaAs-NWs on GaP(111)B using the Au-assisted vapor-liquid-solid growth mode in a metal-organic vapor phase apparatus. Prior to the actual growth, diethylzinc as Zn precursor source is offered for several minutes, so that the Au-particle is saturated with Zn and the NW is doped from beginning of the growth. For electrical characterization these free-standing NWs were contacted using a multitip STM allowing us to measure the resistivity via four-point probe measurements over nearly the complete length of a NW. These measurements reveal a constant resistivity after 1.5 μm NW growth, while it is significantly increasing towards the NW bottom.

O 23: Graphene: Electronic Properties and Transport (jointly with HL, MA and TT)

Time: Monday 16:00–19:00 Location: H17

O 23.1 Mon 16:00 H17

Epitaxial silicene - tunable hybridization with the substrate and weak interactions with epitaxial organic overlayers — •Rainer Friedlein[1], Antoine Fleurence[1], Fabio Bussolotti[1,2], and Yukiko Yamada-Takamura[1] — [1]School of Materials Science, Japan Advanced Institute of Science and Technology (JAIST), Nomi, Ishikawa 923-1292, Japan — [2]present address: Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan

The electronic and structural properties of epitaxial silicene formed on ZrB$_2$(0001) thin films grown on Si(111) wafers upon adsorption of either potassium atoms and anthracene molecules have been studied using photoelectron spectroscopy and electron diffraction. For pristine silicene, a particular, atomic-scale buckling leads to the opening of a direct band gap at the Γ point, while ZrB$_2$-related surface states are not affected. This is consistent with only a minor degree of hybridization beweeen Si- and Zr-derived states. The electronic interactions at the interface can be tuned by electron donation from adsorbed potassium atoms, upon which hybridization is progressively switched on.

At 140 K, anthracene molecules are found to grow as epitaxial multilayers that exhibit a point-on-line commensurate relationship with silicene. The results indicate that the charge-density modulation associated with the buckling of silicene render the interactions with organic adsorbates as compared to graphene, which allows for specific epitaxial conditions. On the other hand, the results also confirm that silicene is strikingly different from other Si surfaces for which the presence of dangling bonds leads to chemisorption of organic adsorbates.

O 23.2 Mon 16:15 H17

***Ab initio* study of graphene nano domes on Ir(111) surface** — •Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, in a combined experimental and theoretical work we have unveiled the bonding mechanism of graphene on Ir(111) surface as physisorption with a local chemical modulation [1]. In this contribution we extend our previous density functional theory (DFT) study to analyse the bonding of graphene nano domes on a clean and an oxygen pre-covered Ir(111) substrate.

As previously shown [1], the inclusion of the long-range van der Waals interactions is mandatory and in our *ab initio* study these dispersion interactions were considered at a semi-empirical [2] or first-principle [3] level, the latter as implemented in our real-space JuNoLo code [4]. In particular, the non-local correlation vdW-DF functional [3] provides an unique visual insight on the origin of a different graphene bonding on Ir(111) due to a non-local and a semi-local description of the correlation effects in DFT.

[1] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).
[2] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).
[3] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).
[4] P. Lazić *et al.*, Comp. Phys. Commun. **181**, 371 (2010).

O 23.3 Mon 16:30 H17

Effects of strain on the excitonic Fano resonance in the optical spectrum of graphene — •Daniela Ullrich[1,2], Patrick Herlinger[1], Harald Giessen[2], Jurgen Smet[1], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]4th Physics Institute, University of Stuttgart

Using transmission and reflection spectroscopy we examine the optical response of graphene from the visible to the UV regime. The absorbance spectrum of free-standing graphene is dominated by an asymmetric peak in the UV at about 4.7 eV. We show that this resonance can be described by a simple Fano model which includes an excitonic state beneath the saddle point of graphene's band structure [1]. When strain is applied to a graphene sheet, the symmetry of the lattice and thus also of the band structure is broken. As predicted recently [2], this should result in a splitting of the absorbance peak in the optical spectrum as well as a strong dependence on polarization and lattice orientation. Here, we present our findings on the effects of strain on the Raman and reflectivity spectra of graphene on flexible substrates.

[1] Chae et al., Nano Lett. 11, 1379 (2011)
[2] Liang et al., J. Mater. Res. 27, 403 (2012)

O 23.4 Mon 16:45 H17

Probing Hot Electron Distributions in Graphene on Ni(111) with High Harmonic Radiation — •Carsten Winter[1], Thorben Haarlammert[1], Luca Bignardi[2], Petra Rudolf[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster — [2]Zernike Institute for Advanced Materials, University of Groningen

Theoretical calculations and experimental observations of hot electron distributions in graphene show an initial ultrafast carrier relaxation accompanied by a population of optical phonons, which decay on a picosecond time scale. In this talk we present an experimental set-up suited to measure the lifetime of excited electrons and their relaxation dynamics via time-resolved 2PPE. Through frequency conversion by High Harmonic Generation coherent radiation at 39 eV photon energy is generated and subsequently used as the probe pulse in two-photon photoemssion.

A graphene sheet was produced by decomposition of ethylene on a Ni(111) substrate. Hot electron distributions were generated in graphene on Ni(111) by applying 800nm pulses. The energy dependent lifetimes of these distributions have been measured. The lifetimes have been determined to 20-50 fs in the lower energy parts of the distribution (E-E$_F$ < 1eV) and show a strong Ni-like behavior. In the upper energy parts lifetimes of 10-20 fs have been measured and a graphite-like behavior dominates.

O 23.5 Mon 17:00 H17

Reversible Photooxidation of Graphene — •Stefan Böttcher, Hendrik Vita, and Karsten Horn — Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany

Graphene oxide is often discussed in the context of a technical usage of graphene in future electronic devices. The necessity to obtain a tunable band gap in possible electronic applications makes graphene oxide a promising covalent modification of graphene. However, the homogeneous preparation of graphene oxide has so far been a challenging task, using mainly an aggressive chemical or complex physical treatment of graphene. Here we present a method to selectively produce graphene oxide from epitaxially grown graphene on transition metal surfaces such as Ir(111). Using NO$_2$ as an adsorbate we transform graphene into graphene oxide by irradiation with UV light at low temperatures, leading to specific signatures in the core and valence level photoemission and -absorption spectra. The graphene oxide thus prepared is stable up to room temperature, but its formation is thermally completely reversible to graphene at higher temperatures.

O 23.6 Mon 17:15 H17

Edge charge disorder in graphene — •Cornelie Koop, Manuel Schmidt, and Carsten Honerkamp — Institut für Theoretische Festkörperphysik, RWTH Aachen University, Deutschland

We study the interplay of edge roughness and electron-electron interaction in graphene nanoribbons. Our focus is the charge response of a rough edge to (possibly random) potentials induced by adatoms. While the bulk density response in graphene is rather small due to the vanishing density of states at the charge neutrality point, it turns out that edges show a strongly increased response - a fact that may be traced back to the presence of localized states at rough edges. The existence of these localized states depends on the structural properties of the edge. They are the disordered analogs to the well known edge states in clean zigzag ribbons and lead to a random sequence of peaks in the local density of states along the rough edge. As a consequence there may be strongly localized charges randomly distributed along the edge. We discuss the conditions for this effect, which we call edge charge disorder, its strength, and its consequences on the bulk electrons in a graphene nanoribbon.

O 23.7 Mon 17:30 H17

Electronic and magnetic properties of zigzag graphene nanoribbons on the (111) surface of Cu, Ag and Au — •Yan Li[1], Wei Zhang[1], Markus Morgenstern[2], and Riccardo Mazzarello[1] — [1]Institute for Theoretical Solid State Physics and JARA, RWTH Aachen University, D-52074 Aachen, Germany — [2]II. Physikalisches Institut B and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany

We have carried out an *ab initio* study of the structural, electronic and magnetic properties of zigzag graphene nanoribbons (GNRs) on Cu(111), Ag(111) and Au(111). Both H-free and H-terminated GNRs are considered revealing that the nanoribbons invariably possess edge states when deposited on these surfaces. In spite of this, they do not exhibit magnetism at the edge, with the exception of H-terminated GNRs on Au(111), whose zero-temperature magnetic properties are comparable to those of free-standing GNRs. The absence of edge magnetism is due to the hybridization between the $2pz$ orbitals of the carbon atoms and the d states of the metal and, for some models, to the charge transfer between the GNR and the surface, which shifts the edge state away from the Fermi level. Only in the case of H-terminated GNRs on Au(111) is the interaction between the substrate and the GNR sufficiently weak so as not to affect the magnetic properties of the edge state significantly.

O 23.8 Mon 17:45 H17

The atomic and electronic structure of well-defined graphene nanoribbons studied by scanning probe microscopy — •Joost van der Lit[1], Mark Boneschanscher[1], Mari Iljas[2], Ari Harju[2], Andreas Uppstu[2], Daniel Vanmaekelbergh[1], Peter Liljeroth[2], and Ingmar Swart[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands — [2]Department of Applied Physics, Aalto University, Finland

Recently, graphene nanostructures have gained a lot of interest since they introduce a bandgap in graphene, which is important for (opto-) electronics applications. Graphene nanoribbons can have a bandgap as large as 3 eV[1,2], which can be tuned by varying its width. By using a chemical bottom-up approach, we have synthesized graphene nanoribbons (GNR) on an Au(111) substrate[3]. By combining scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with reactive and non-reactive tips, we can relate the electronic properties of the GNRs with their atomic structure. Furthermore, we can use the STM tip to (i) deliberately create well-defined atomic scale defects and (ii) control the interaction with the substrate. Hence, we are able to directly study the robustness of the properties of the graphene nanostructures. [1] P. Ruffieux, et al. , ACS Nano 6 (2012) 6930. [2]M. Koch, F. Ample, C. Joachim, L. Grill, Nat. Nanotechnol. 7 (2012)713. [3] J. Cai et al., Nature, 446 (2010) 470-473.

O 23.9 Mon 18:00 H17

Intact Dirac cones at broken sublattice symmetry: photoemission study of graphene on Ni and Co — •Dmitry Marchenko[1], Andrei Varykhalov[1], Jaime Sánchez-Barriga[1], Markus R. Scholz[1], Bart Verberck[2], Björn Trauzettel[3], Tim O. Wehling[4,5], Carlo Carbone[6], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Universiteit Antwerpen — [3]Universität Würzburg — [4]Universität Bremen — [5]Bremen Center for Computational Materials Science — [6]Consiglio Nazionale delle Ricerche Trieste

A band gap at the Dirac point of graphene can be created by breaking of the sublattice symmetry through epitaxial growth on a substrate crystal. One of the strongest sublattice-symmetry-breaking interactions with predicted and measured band gaps ranging from 400 meV to more than 3 eV has been attributed to the interfaces of graphene with Ni and Co, which are also promising spin filter interfaces. We apply angle-resolved photoemission to epitaxial graphene on Ni(111) and Co(0001) to show the presence of intact Dirac cones in a strongly n-doped system. Our results challenge the common belief that breaking of sublattice symmetry by a substrate and opening of the band gap at the Dirac energy are in a straightforward relation. A simple effective model of a biased bilayer structure composed of graphene and a sublattice symmetry broken layer, corroborated by density functional theory calculations, demonstrates the general validity of our conclusions.

O 23.10 Mon 18:15 H17

sp^2 carbon hybrid junctions — Pablo Robert[1,2], Renjun Du[1], Fan Wu[1], Kristina Hönes[1], Jens Mohrmann[1], Frank Hennrich[1], Manfred Kappes[1,3,4], Hilbert von Löhneysen[1,2,4,5], and •Romain Danneau[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, — [2]Institute of Physics, Karlsruhe Institute of Technology, Germany — [3]Institute of Physical Chemistry, Karlsruhe Institute of Technology, Germany — [4]DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, Germany — [5]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Germany

Lowering the contact resistance is a key issue to improve graphene field effect device performance. The connection between a metal and graphene depends on many parameters such as the work function mismatch between the two connected material, the adsorption of the metal on graphene, the quality of the deposited material as well as the strain induced on the graphene sheet. We have studied electronic transport through carbon nanotube (CNT)-graphene and graphene-graphene junctions produced by nano-manipulation and transfer. For the CNT-graphene junctions, we first demonstrate that the influence of the CNT on the charge distribution of the graphene sheet is limited to few nanometers. Our experiments show that the junction transparency is strongly gate dependent due to the variation of the CNT-graphene distance, and the charge carrier injection occurs via a single point. For the graphene-graphene junctions, our measurements show low resistance and prove that graphene makes a good connection to graphene.

O 23.11 Mon 18:30 H17

Graphene on boron nitride microwave transistors driven by graphene nanoribbon back-gates — Christian Benz[1,2], •Maximilian Thürmer[1], Fan Wu[1], Zeineb Ben Aziza[1], Jens Mohrmann[1], Hilbert von Löhneysen[1,2,3,4], Kenji Watanabe[5], Takashi Taniguchi[5], and Romain Danneau[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]Institute of Physics, Karlsruhe Institute of Technology, Germany — [3]DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, Germany — [4]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Germany — [5]Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan

We have designed ultra-thin graphene microwave transistors by using pre-patterned metal or graphene nanoribbon back-gates and hexagonal boron nitride (h-BN) as a dielectric substrate. Despite the inhomogeneities induced by the graphene transfer process, we show that it is possible to operate these types of devices across a broad range of microwave frequencies. For the graphene nanoribbon gates, we observe a deviation of the current gain from the usual 1/f trend that can be attributed to the large gate resistance of these systems as we demonstrate with our small-signal model. The scattering parameter analysis shows a very limited back-action from the channel onto the graphene nanoribbon gates. Our work thus proves that graphene microwave transistors could be driven by graphene nanoribbon gates.

O 23.12 Mon 18:45 H17

Strong gate hysteresis in graphene on mica field effect devices — •Jens Mohrmann[1], Kenji Watanabe[2], Takashi Taniguchi[2], and Romain Danneau[1,3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan — [3]Institute of Physics, Karlsruhe Institute of Technology, Germany

One of the outstanding properties of graphene is the unbeatable ratio of surface to volume. As a membrane of only one atomic layer of carbon, graphene is extremely sensitive to external influences. The large area contact with the substrate thus causes a large influence of the used substrate on the electronic properties of graphene. Therefore, a lot of effort is being made in order to understand the interaction between graphene and its substrate, and to find new and possibly better materials. One material under investigation is muscovite mica. The layered structure allows perfect basal (001) cleavage with atomically flat terraces, and using mechanical exfoliation, very thin crystals can be created and used as a substrate and gate dielectric. Transport measurements of graphene on mica show a very high hysteresis with respect to the gate voltage. Here, we investigate this effect using dual gated devices, with both mica and hexagonal boron-nitride dielectrics.

O 24: Organic Electronics and Photovoltaics I (jointly with CPP, DS, HL)

Time: Monday 17:15–18:45 Location: H32

O 24.1 Mon 17:15 H32

Correlation between interface energetics and open circuit voltage in organic photovoltaic cells — •Andreas Wilke[1], James Endres[2], Ulrich Hörmann[3], Jens Niederhausen[1], Raphael Schlesinger[1], Johannes Frisch[1], Patrick Amsalem[1], Julia Wagner[3], Mark Gruber[3], Andreas Opitz[1], Antje Vollmer[4], Wolfgang Brütting[3], Antoine Kahn[2], and Norbert Koch[1,4] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 15, D-12489 Berlin, Germany — [2]Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, USA — [3]Universität Augsburg, Institut für Physik, Universitätsstr. 1, D-86135 Berlin, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH BESSY II, Albert-Einstein-Str. 15, D-12489 Berlin, Germany

We have used ultraviolet and inverse photoemission spectroscopy to determine the transport gaps (E_T) of C60 and diindenoperylene (DIP), and the photovoltaic gap (E_PVG) of five prototypical donor/acceptor interfaces used in organic photovoltaic cells (OPVCs). The transport gap of C60 (2.5 ± 0.1) eV and DIP (2.55 ± 0.1) eV at the interface is the same as in pristine films. We find nearly the same energy loss of ca. 0.5 eV for all material pairs when comparing the open circuit voltage measured for corresponding OPVCs and E_PVG.

O 24.2 Mon 17:30 H32

Direct Observation of Charge Separation in Perylene Monoimide Solid State Dye-Sensitized Solar Cells — •Ian Howard[1], Michael Meister[1], Björn Baumeier[1], Henrike Wonnenberger[1], Neil Pschirer[2], Rüdiger Sens[2], Ingmar Brüder[2], Klaus Müllen[1], Denis Andrienko[1], and Frédéric Laquai[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — [2]BASF SE

Combining Vis-NIR broadband pump-probe transient absorption spectroscopy with precise measurement of the time-resolved photoinduced Stark effect we demonstrate that it is possible to track not only the rate of charge injection but also the motion of carriers after injection on the critical nanosecond timescale in Solid State Dye Sensitized Solar Cells. In terms of solar cell efficiency our findings have two major impacts. Firstly, we directly observe that the *reductive quenching* pathway previously suggested (wherein a photoexcited dye donates a hole to the hole transport material before then injecting an electron, now from the dye anion state, into the TiO2) is important for obtaining high device efficiencies, especially for NIR absorbing dyes which exhibit a reduced driving force for electron injection directly from the dye exciton. Secondly, we find that many charges return to the interface after following injection, likely due to Coulombic and image charge effects. Screening the charges better, for example by reducing the dielectric contrast or increasing the dye length, should decrease the interfacial charge density and thereby parasitic recombination.

O 24.3 Mon 17:45 H32

Full electronic structure across a polymer heterojunction solar cell: interface dipoles and influence of light — •Johannes Frisch[1], Patrick Amsalem[1], Jens Niederhausen[1], Marcel Schubert[2], Eduard Preis[3], Antje Vollmer[4], Jürgen P. Rabe[1], Ullrich Scherf[3], Dieter Neher[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]Universität Potsdam, Germany — [3]Bergische Universität Wuppertal, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie - Speicherring BESSY II, Berlin, Germany

Controversial discussions concern the dependence of open circuit voltage on the energy offset between the highest occupied molecular orbital level of the donor material and the lowest unoccupied molecular orbital level of the acceptor material in organic photovoltaic cells. Therefore, we investigate the energy level alignment in two bilayer OPVCs comprising the donor poly(3-hexylthiophene) (P3HT) and the acceptors 1-(3-methoxycarbonyl)propyl-1-phenyl[6.6]C61 (PCBM) and poly(9,9'dialklylfluorene-alt- 4,7-bis(2,5-thiendiyl)-2,1,3-benzothiadiazole) (PFTBTT). Ultraviolet photoelectron spectroscopy revealed that notable interface dipoles occur at all interfaces across the OPVC structures for both material combinations. Particularly, the effective electrode work function (after contact formation with the organic material) differs significantly from those of the pristine materials. In addition, we find that negative charges are collected at the metal clusters (that exist in the early stage of cathode formation) due to exciton dissociation at the heterojunction.

O 24.4 Mon 18:00 H32

Optoelectronic Properties Of Zinc(II)-Phthalocyanine — •Michael Kozlik, Sören Paulke, Marco Gruenewald, Roman Forker, and Torsten Fritz — University of Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

Zinc phthalocyanine (ZnPc) is an organic molecule which is used in organic optoelectronic devices, such as OLEDs and organic solar cells. Bulk material is represented mainly in form of the metastable α-ZnPc, while the stable β-ZnPc is less conductive [1]. We show the critical transformation temperature as well as optical and morphological differences between both phases. Description and simulation of the performance of organic devices make use of material parameters. In our work we present the determination of the optical constants and the exciton diffusion length. Experimental methods are UV-Vis spectroscopy and external quantum efficiency. By transmittance and reflectance spectra we derive the real and imaginary part of the refractive index [2]. In combination with the derived parameters we show the performance of a simplified photovoltaic cell and identify the region of exciton dissociation and exciton diffusion length.

References

[1] K. Wihksne et al., J. Chem. Phys. 34 (1961) 2184.

[2] M. Kozlik et al., Org. Electron. 13 (2012) 3291.

O 24.5 Mon 18:15 H32

The operational mechanism of ionic transition metal complex-based light-emitting electrochemical cells — •Sebastian B. Meier[1,2], Stephan van Reenen[3], Henk J. Bolink[4], Martijn Kemerink[3], Wiebke Sarfert[2], and Albrecht Winnacker[1] — [1]Department of Materials Science VI: Materials for Electronics and Energy Technology, University of Erlangen-Nuremberg, Germany — [2]Siemens AG, Corporate Technology, CT RTC MAT MPV-DE, Erlangen, Germany — [3]Department of Applied Physics, Eindhoven University of Technology, The Netherlands — [4]Instituto de Ciencia Molecular, Universidad de Valencia, Spain

Light-emitting electrochemical cells (LECs) are promising candidates for cost-efficient next generation solid-state lighting and signage applications. They feature only a single, solution-processible active layer comprising a luminescent material in an ionic environment which allows for charge carrier injection from air-stable electrodes and low operating voltages. The operational mechanism of LECs has been the subject of an intense debate ever since their discovery. Evidence for electrochemical doping has been demonstrated for polymer-based devices, whereas LECs comprising ionic transition metal complexes (iTMCs) have almost exclusively been stated to operate via an electrodynamic mechanism. We used fluorescence as well as scanning Kelvin probe microscopy on planar iTMC-LECs to elucidate their mechanism of work. Our results illustrate profound evidence for electrochemical doping in these kind of LEC devices and highlight that the position of the established p-i-n junction is not fixed but migrates during device operation.

O 24.6 Mon 18:30 H32

Effective Charge Carrier Lifetimes in Organic Solar Cells Prepared by Coevaporation of $C60$ and $CuPc$ in different mixtures and geometries — •André Dragässer and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Giessen, Germany

Evaporated organic solar cells can lead to efficiencies of technical relevance if the interface of donor and acceptor molecules is optimized for the interplay of exciton dissociation, charge transport and recombination. The effective lifetime of the charge separated state is of central relevance. Intensity- modulated photovoltage spectroscopy with parallel impedance spectroscopy is a suitable method of analysis. Organic solar cells consisting of the well-established semiconductor materials $CuPc$ and $C60$ were prepared by physical vapor deposition on an ITO substrate, modified with $PEDOT : PSS$. The cells were completed by a back contact of BCP as a buffer and aluminum. Cell architectures of planar junctions, bulk heterojunctions or planar-mixed heterojunctions were studied for different film thickness of the components. IV-measurements in the dark and under varied illumination intensities provided basic device characteristics. Detailed measurements of the short-circuit photocurrent and the open-circuit photovoltage under static or intensity-modulated illumination with different wavelength were performed to determine the average charge carrier lifetime in the devices which was related to the respective charge carrier density obtained by impedance spectroscopy. Recombination reactions and, in particular, the influence of trap states will be discussed.

O 25: Invited Talk (Sohrab Ismail-Beigi)

Time: Tuesday 9:30–10:15 Location: H36

Invited Talk O 25.1 Tue 9:30 H36

Flippable charge, magnetic, and orbital modulation at ferroelectric/manganite interfaces from first principles — •Sohrab Ismail-Beigi — Department of Applied Physics, Yale University

We discuss recent first principles theoretical work on transition metal oxide interfaces involving ferroelectrics and manganites. We describe how the ferroelectric polarization has multiple effects on the interfacial region of the conducting manganite in that it modifies the electron distribution, changes the magnetic phase, and also reorders the energies of the key electronic orbitals (i.e. orbital polarization). Since the polarization of a ferroelectric has two states, these interfacial properties are dynamically flippable by using an electric field to flip the ferroelectric polarization. We describe which of the physical phenomena can be understood from bulk properties and which are genuinely interfacial and represent phases not possible in bulk manganites. In the process, we also describe the challenges in modeling such manganite systems with state-of-the-art methods such as density functional theory (DFT) and the DFT+U approach.

O 26: Transport: Graphene - Electronic Properties and Transport 2 (jointly with DS, HL, MA, and TT)

Time: Tuesday 9:30–12:45 Location: H17

O 26.1 Tue 9:30 H17

Transport properties of high-quality reduced graphene oxide — •Michael Enzelberger[1], Siegfried Eigler[2], Philipp Hofmann[1], Stefan Grimm[2], Andreas Hirsch[2], and Paul Müller[1] — [1]Department of Physics and Interdisciplinary Center for Molecular Materials, Universität Erlangen-Nürnberg — [2]Department of Chemistry and Pharmacy, and Institute of Advanced Materials and Processes (ZMP), Universität Erlangen-Nürnberg

Chemical production of graphene, especially reducing graphene oxide has gained a lot of interest in recent years. Yet the transport properties of such materials are usually not compatible to those of graphene.

We have found a way to overcome this problem using a modification of the standard Hummer's method. Single flakes of reduced graphene oxide have been investigated. The graphene oxide was deposited onto a SiO_2/Si substrate and subsequently reduced using hydrogen iodine. The resulting reduced graphene oxide samples were patterned by electron beam lithography. We have characterized the quality of the samples by combining Raman spectroscopy and Hall mobility measurements in magnetic fields up to $14\,T$ and temperatures down to $0.3\,K$.

High-quality samples had a Raman D/G ratio of better than 1 and showed Hall mobilities exceeding 1000 cm^2/Vs. This is nearly two orders of magnitude higher than what is known for standard reduced graphene oxide. The best samples even show Shubnikov-de Haas oscillations and Hall plateaus.

O 26.2 Tue 9:45 H17

Magnetoresistance of Nanocrystalline Graphene — •Daniel Steininger[1], Paul Linsmaier[1], Ina Schneider[1], Christoph Strunk[1], Matthias Büenfeld[2], Nils-Eike Weber[2], Andrey Turchanin[2], Miriam Grothe[3], and Thomas Weimann[3] — [1]Institute for Experimental and Applied Physics, University of Regensburg, Universitätsstr. 31, D-93053 Regensburg, Germany — [2]Faculty of Physics, University of Bielefeld,Universitätsstr.25, D-33615 Bielefeld, Germany — [3]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

We report on the magnetotransport in Hall bar structures of nanocrystalline graphene. The graphene sheets were prepared by electron-beam-induced cross-linking and subsequent pyrolysis of aromatic self-assembled monolayers [1]. The I-V characteristics show considerably non-linear behaviour at low temperatures. One low resistive sample ($\approx$ 200 kOhm/sq at T = 4 K) shows positive magnetoresistance values up to + 20 % in the perpendicular magnetic field for temperatures below 6 K, while above this temperature the magnetoresistance becomes negative. Measurements of the transversal voltage in the linear regime exhibit anomalous behaviour which cannot be explained by the conventional Hall effect. If the magnetic field is aligned parallel to the graphene sheet the magnetorestance exhibits large positive values up to + 300 %. Measurements on a highly resistive sample ($\approx$ 30 MOhm/sq at T = 4 K) reveal a non-monotonic behaviour of the magnetoresistance in a perpendicular magnetic field.

[1] A. Turchanin et al., ACS Nano 5 (2011) 3896-3904.

O 26.3 Tue 10:00 H17

Quantum Monte Carlo Study of Edge-State Magnetism on Chiral Graphene Nanoribbons — Michael Golor[1], Thomas C. Lang[1,2], and •Stefan Wessel[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen — [2]Department of Physics, Boston University

We investigate the edge-state magnetism of chiral graphene nanoribbons using projective Quantum Monte Carlo (QMC) simulations and a self-consistent mean-field approximation of the Hubbard model. Previous QMC simulations support edge-state ferromagnetism in sufficiently wide zigzag terminated ribbons. We extended these calculations to include the class of chiral graphene nanoribbons and investigate the influence of chirality and ribbon width on spin-spin correlations. The static magnetic correlations are found to rapidly increase with the width of the ribbons for all chiralities, such that already for ribbons of moderate widths we observe a strong trend towards mean-field-type ferromagnetic correlations along the edges. We extract dynamical edge state signatures which can be used to detect edge-state magnetism by scanning tunneling microscopy.

O 26.4 Tue 10:15 H17

Even-odd effects in NSN scattering problems: Application to graphene nanoribbons — •Francois Crepin[1], Hans Hettmansperger[1], Patrik Recher[2], and Bjoern Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Wuerzburg, 97074 Wuerzburg, Germany — [2]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

We study crossed Andreev reflection (CAR) of electrons or holes in normal metal-superconductor-normal metal junctions and highlight some very strong effects of the underlying lattice. In particular, we demonstrate that for sharp interfaces and under certain, albeit generic, symmetry conditions, the CAR probability exactly vanishes for an even number of atoms in the superconducting region. This even-odd effect applies notably to NSN junctions made of graphene nano-ribbons with armchair edges and for zigzag edges with somewhat more restrictive conditions. We analyze its robustness towards smoothing of the boundaries or doping of the sample.

O 26.5 Tue 10:30 H17

Efficient quantum transport simulation for bulk graphene heterojunctions: Klein backscattering revisited — •Ming-Hao Liu and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

The quantum transport formalism based on tight-binding models is known to be powerful in dealing with a wide range of open physical systems subject to external driving forces but is, at the same time, limited by the memory requirement's increasing with the number of atomic sites in the scattering region. Here we demonstrate how to achieve an accurate simulation of quantum transport feasible for experimentally sized bulk graphene heterojunctions at a strongly reduced computational cost [1]. Without free tuning parameters, we show excellent agreement with recent experiments on Klein backscattering [2,3].

[1] M.-H. Liu and K. Richter, Phys. Rev. B **86**, 115455 (2012).
[2] A. F. Young and P. Kim, Nat. Phys. **5**, 222 (2009).
[3] S.-G. Nam, D.-K. Ki, J. W. Park, Y. Kim, J. S. Kim, and H.-J. Lee, Nanotechnology **22**, 415203 (2011).

O 26.6 Tue 10:45 H17

Combined effect of vacancies and strain on the conductance of graphene nanoribbons — •Thomas Lehmann, Dmitry A. Ryndyk, and Gianaurelio Cuniberti — Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany

The understanding and engineering of electron properties of carbon-based nanostructures, in particular graphene nanoribbons, is an important challenge for modern theory of nanoscale systems. We investigate the influence of vacancy defects and uniaxial strain on the electronic transport properties of intermediate-scale graphene nanoribbons using the numerical approach based on the semi-empirical or ab initio based tight-binding model, the Landauer-Büttiker formalism and the recursion method for Green functions. We calculate the transmission of graphene nanoribbons in the quantum coherent regime with different types and concentration of defects. Further, we apply uniform planar tension to non-ideal graphene ribbons with randomly distributed and oriented single and double vacancies and Stone-Wales defects. Since transport characteristics of graphene are found to be very sensitive to edge termination and aspect ratio and it has been shown that energy gaps can emerge under critical strain, the interplay of both effects needs to be studied.

15 min. break

O 26.7 Tue 11:15 H17

Spin conductance of diffusive graphene nanoribbons — •Jan Bundesmann[1], Ming-Hao Liu[1], Inanc Adagideli[2], and Klaus Richter[1] — [1]University of Regensburg, Regensburg, Germany — [2]Sabanci University, Istanbul, Turkey

Graphene, when cut along a zigzag edge, shows a strongly increased density of states at energies close to the charge neutrality point. The electron states that are the source of this increased DOS are pseudospin-polarized, i.e. they occupy mainly one sublattice, while their wavefunction decays exponentially from the zigzag edge.

In such systems one expects magnetic ordering which anifests as an antiferromagnetic alignment of the two sublattices. Due to the pseudospin polarization of the states finite local magnetic moments appear along the edges.

We investigate how the formation of these local magnetic moments influences charge and spin transport in graphene. It will be shown how this can lead to a finite spin conductance of a single graphene nanoribbon and that within the localized transport regime the spin conductance fluctuations exhibit universal behaviour in the sense that they don't depend on the exact modelling of the magnetization and even a large amount of edge roughness does not lead to deviations from this universal behaviour.

O 26.8 Tue 11:30 H17

Superlattice Effects on Electronic- and Transport Properties of Nanomaterials — •Fedor Tkatschenko, Viktor Krueckl, and Klaus Richter — Universität Regensbug, Germany

As recently discoverded by various groups [1,2] the electronic properties of two dimensional systems such as graphene show interesting characteristics in presence of superlattices including the emergence of extra Dirac points accompanied by an anisotropic velocity renormalization. Other interesting effects are Bloch-oscillations in presence of resonant Zener tunneling [3] giving rise to a negative differential conductance in the current voltage characteristics.

We focus on a scalar superlattice system extended by a constant mass term which opens a gap between the valance and conduction band in the minibandstructure. Analytical calculations within the effective Dirac model show that it is possible to tune the energy gap by variation of the superlattice amplitude. By additional numerical calculations based on the tight-binding model we confirm the analytical results.

[1] L. Brey and H. Fertig, Phys. Rev. Lett. **103**, 046809 (2009)
[2] M. Barbier, P. Vasilopoulos, and F. Peeters, Phys. Rev. B **81**, 075438 (2010)
[3] V. Krueckl and K. Richter, Phys. Rev. B **85**, 115433 (2012)

O 26.9 Tue 11:45 H17

Hot Spots and Boundary Conditions in the Quantum Hall Effect — •Tobias Kramer — Universitaet Regensburg, Inst. Theor. Physik, Germany

I discuss the influence of metallic boundary conditions due to the device contacts on the observation and current distribution in the quantum Hall effects. The current density differs in the presence of hot-spots completely from the often assumed edge-state transport picture. A model for transport in graphene [1] based on the self-consistent solution of the classical Hall effect [2] is put forward.

[1] T. Kramer, C. Kreisbeck, V. Krueckl, E. Heller, R. Parrott, and C.-T. Liang, Phys. Rev. B **81**, 081410(R) (2010)
[2] T. Kramer, V. Krueckl, E. Heller, and R. Parrott, Phys. Rev. B **81**, 205306 (2010)

O 26.10 Tue 12:00 H17

Current resonances in graphene with time dependent potential barriers — Sergey E. Savel'ev[1], •Wolfgang Häusler[2], and Peter Hänggi[2] — [1]Department of Physics, Loughborough University, United Kingdom — [2]Universität Augsburg, Germany

A method is derived to solve the massless Dirac-Weyl equation describing electron transport in a mono-layer of graphene with a scalar potential barrier $U(x,t)$, homogeneous in the y-direction, of arbitrary x- and time dependence. Resonant enhancement of both electron backscattering and currents, across and along the barrier, is predicted when the modulation frequencies satisfy certain resonance conditions. These conditions resemble those for Shapiro-steps of driven Josephson junctions. Surprisingly, we find a non-zero y-component of the current for carriers of zero momentum along the y-axis.

[1] Sergey E. Savel'ev, Wolfgang Häusler, Peter Hänggi, Phys. Rev. Lett. **109**, 226602 (2012).

O 26.11 Tue 12:15 H17

Mie scattering analogon in graphene: particle confinement, scattering resonances, and Fano effect — •Rafael Leslie Heinisch, Christian Schulz, Franz Xaver Bronold, and Holger Fehske — Institut für Physik, Universität Greifswald

We study the scattering of an incident electron by a circular step in a graphene monolayer in analogy to Mie scattering of light by a sphere. Klein tunnelling results in the absence of backscattering and often entails enhanced forward scattering. For low electron energies we identify sharp resonances originating from quasi-bound states at the dot. The energy and dot radius dependent temporary electron trapping significantly increases the electron density in the dot and induces a vortex pattern in the current field. The angle-resolved scattering exhibits Fano resonances which - counter-intuitive for Klein tunnelling - dramatically suppress forward scattering.

This work is supported by the DFG through SPP 1459.

O 26.12 Tue 12:30 H17

Mechanical strain on graphene nanoribbons in contact with metal electrodes — •Arezoo Dianat, Dmitry A. Ryndyk, and Gianaurelio Cuniberti — Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany

Carbon-based materials are recently of great interest for electronic devices. One of the important issues in graphene based nanoelectronics is to control its electronic and transport properties. The manipulation of electronic properties of graphene nanoribbons (GNR) has been suggested via mechanical strain, vacancies and chemical doping. From modeling point of view, few studies have been reported to investigate the electronic properties of mechanically stretched GNR in a contact with metal electrodes. In this work, we aim to elucidate the combined effects of mechanical strain and the role of metal contact area on the electronic and transport properties of GNR.

The structural and electronical properties of stretched GNR on Nickel and Palladium surfaces with different contact area and suspended strained graphene junction between metal electrodes are investigated by means of density functional theory using Vienna Ab initio Simulation Package (VASP). The structure stability as well as stress-strain curve are analyzed for several strain coefficients.

O 27: Organic Electronics and Photovoltaics II (jointly with CPP, DS, HL)

Time: Tuesday 9:30–12:45 Location: H32

O 27.1 Tue 9:30 H32

Influence of triplet excitons on the lifetime of polymer based organic light emitting diodes — •Oili Pekkola, Andrea Gassmann, Christian Melzer, and Heinz von Seggern — Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

Despite the promising development of polymer based organic light emitting diodes (PLEDs), device lifetime and stability are still among the most critical issues. One of the lifetime-related factors investigated to a lesser extent is the influence of the high density of non-emissive triplet excitons which could be responsible for local heating or act as traps for charge carriers, leading to a degradation of the device.

This study utilizes PLEDs based on poly(p-phenylene vinylene) (PPV) derivatives to understand the influence of triplet excitons on the fatigue by increasing their amount in the PPV film. This increase is achieved by blending different concentrations of the triplet sensitizer platinum (II) octaethylporphine ketone (PtOEPK) into the PPV matrix in order to convert PPV singlet excitons to triplets. One observes that in PLEDs both the t50 and t90 lifetimes are drastically shortened in the presence of PtOEPK. To rule out a possible influence of the sole presence of PtOEPK on charge carrier transport, single carrier devices with different sensitizer contents were prepared. In these devices, no fatigue is observed regardless of the sensitizer concentration, suggesting that the decrease in the lifetimes of the bipolar diodes is indeed caused by the increased triplet population in the diodes with sensitized polymer films and not by the sensitizer additive as such.

O 27.2 Tue 9:45 H32

Homogeneity of thin ZnTPP-films on silicon measured with reflectance anisotropy spectroscopy and Raman spectroscopy — •Stephan Peter Kate[1], Simona Pop[1], Jörg Rappich[2], and Karsten Hinrichs[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein Str. 9, Berlin, 12489 Germany — [2]Helmholtz-Zentrum for Materials and Energy GmbH, Kekulestraße 5, Berlin, 12489, Germany

Organic devices for electronic applications are an important field of research. To improve the efficiency of those components, the analysis of structure and homogeneity of thin films is of crucial importance. In this study we demonstrate that Reflectance Anisotropy Spectroscopy (RAS) and Raman spectroscopy are useful to investigate the homogeneity of thin films of zinc-tetra-phenyl-porphyrin (ZnTPP) on silicon substrates. The RAS spectra of the thin films show an optical anisotropy in the visible spectral range. Analyzing the anisotropy, conclusions about the homogeneity of the thin films can be drawn. The vibrational modes of the molecules seen with resonant Raman spectroscopy are sensitive to the film structure. A pyrrole-bending mode in the region of 1075 cm-1 serves us as a marker for the film homogeneity. The RAS and Raman results are correlated with AFM measurements.

O 27.3 Tue 10:00 H32

Morphology evolution of diblock copolymer based ZnO nanostructures upon solvent vapor treatment — •Kuhu Sarkar, Christoph Schaffer, Anna Naumann, Daniel Mosegui Gonzalez, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Nanostructured inorganic metal oxides with tunable morphologies are desirable for optimizing many potential applications in the field of gas/chemical sensing, catalysis and energy storage. Zinc oxide (ZnO) is chosen in the present study owing to its outstanding optical and electrical properties. Different ZnO nanostructures are synthesized using a suitable diblock copolymer template via sol-gel chemistry. Zinc acetate dihydrate is used as the suitable commercial precursor for ZnO. There are several possibilities to tune the morphology as most of the diblock copolymers respond to the external fields such as temperature and solvent vapor. Hence, tetrahydrofuran solvent vapor treatment has been employed to the as-prepared thin films corresponding a grid-like morphology for different annealing times. Grazing incidence small angle X-ray scattering (GISAXS) has been performed to probe the structural order over the entire film volume. Evolution of the morphology has been followed by GISAXS studies as a function of different solvent treatment times. The annealed films are subsequently calcined at a higher temperature in order to understand the preservation of higher orders in the ZnO structure even after removal of the diblock copolymer.

O 27.4 Tue 10:15 H32

Correlation of morphology and electronic properties of MoO_3 doped CBP layers I: TEM and electrical properties — •Daniela Donhauser[1,2], Levin Dieterle[1,2], Paul Heimel[3,2], Tobias Glaser[3,2], Maybritt Kühn[4,2], Mustapha Al-Helwi[5,2], Rasmus R. Schröder[6], Eric Mankel[4,2], Michael Kröger[1,2], and Wolfgang Kowalsky[1,2] — [1]Institut für Hochfrequenztechnik, TU Braunschweig, Braunschweig — [2]InnovationLab GmbH, Heidelberg — [3]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg — [4]Institut für Materialwissenschaft, TU Darmstadt, Darmstadt — [5]BASF SE, Ludwigshafen — [6]CellNetworks, Universität Heidelberg

Since electrochemical doping can significantly improve the performance of organic devices, the understanding of the fundamental properties of doped thin films is crucial. For a variety of different material systems a very low doping efficiency was observed, although from energetical considerations a very efficient charge transfer is expected. Using bright-field TEM and electron tomography we show for MoO_3-doped CBP ((4,4'-Bis(N-carbazolyl)-1,1'-biphenyl) thin films that this low doping efficiency is due to filament-like dopant agglomeration which can be controlled by changing the substrate temperature during the evaporation process [1]. The observed morphology is finally correlated with electrical properties like charge carrier density and mobility and depending on the dopant concentration an anisotropic charge transport is observed.

[1] Donhauser et al., Adv. Funct. Mater., 2012, 10.1002/adfm.201202089

O 27.5 Tue 10:30 H32

Correlation of morphology and electronic properties of MoO_3-doped CBP layers II: IR spectroscopic study — •Tobias Glaser[1,5], Sebastian Beck[1,5], Daniela Donhauser[2,5], Maybritt Kühn[3,5], Bernd Lunkenheimer[4,5], Andreas Köhn[4,5], Eric Mankel[3,5], and Annemarie Pucci[1,5] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Technische Universität Darmstadt, Fachbereich Materialwissenschaft, Fachgebiet Oberflächenforschung — [4]Universität Mainz, Institut für Physikalische Chemie — [5]InnovationLab GmbH, Heidelberg

In order to obtain a further understanding on the charge transfer process in p-type doping using transition metal oxides, we performed insitu FTIR-spectroscopy on thin layers of 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP) doped with MoO_3. In the doped layers, charge transfer complexes (CTCs) are formed, that exhibit a broad electronic excitation in the near IR region. These CTCs are located at the interface of the MoO_3 agglomerates and the organic matrix, inducing an interface dipole. The intensity of this electronic excitation in the spectra of layers with various doping concentrations indicates a linear increase of the agglomerates' surface area with MoO_3 concentration. The vibrational changes in the spectra of the doped layers indicate a charge transfer of Z=1e within the CTCs. By cooling the substrate during the deposition process, the agglomeration of the dopants can be suppressed.

Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

O 27.6 Tue 10:45 H32

Correlation of morphology and electronic properties of MoO_3-doped CBP layers III: XPS and UPS study — •Maybritt Kühn[1,4], Eric Mankel[1,4], Daniela

Donhauser[2,4], Tobias Glaser[3,4], Thomas Mayer[1,4], and Wolfram Jaegermann[1,4] — [1]Technische Universität Darmstadt, Fachgebiet Materialwissenschaft — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Universität Heidelberg, Kirchhoff-Institut für Physik — [4]InnovationLab GmbH, Heidelberg

Electro-chemical doping is a prerequisite to improve efficiency and conductivity of organic OLED materials. Here the p-type doping behavior of MoO$_3$ is analyzed using photoelectron spectroscopy (XPS/UPS). The doped CBP layers were evaporated and analyzed under UHV conditions. Concerning the Fermi level shift three different regimes can be distinguished: At low doping concentrations ($< 9\,\mathrm{mol\%}$) a rapid shift towards the HOMO level of CBP can be observed, becoming less strong and finally saturating at a maximum shift of 1 eV at a doping concentration of 45 mol%. The electron transfer from CBP to MoO$_3$ leads to the formation of reduced MoO$_3$. Determining the amount of these species we get information of the surface to volume ratio of the MoO$_3$ clusters in dependence of the doping concentration. Also here three different regimes can be distinguished. The morphology and Fermi level shift regimes will be correlated discussing the dopant morphology as shown in Talk I. Finally the amount of transferred charges is calculated regarding the reduced MoO$_3$ species and is compared with the number of cations determined by IR-spectroscopy (Talk II).

Coffee break (15 min)

O 27.7 Tue 11:15 H32

Organic semiconductor devices on fibre shaped structures for smart textile applications. — •Tobias Könyves-Toth, Andrea Gassmann, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

In the development of smart textiles already realized prototypes utilize embedded LEDs, displays or interactive communication devices based on inorganic semiconductor technology. Yet, these wearable smart textiles are not always comfortable since inorganic devices are stiff and rigid. On the other hand, organic electronic devices can be realized on flexible substrates employing very thin active layers of only about 100 nm thickness. The aim of the present work is to process organic semiconductor based devices directly on fibre surfaces. This task is challenging as manufacturing related problems due to the cylindrical shape of the fibre substrates and their small diameter of about 200 nm have to be overcome. Here, we present our findings on functional OLEDs on fibre substrates. Also the choice of proper fibre materials, ways to acquire smooth fibre surfaces and the structuring and encapsulation of fibre-shaped devices will be discussed. Additionally, methods to characterize the functionality of the devices, like angle dependence emission, will be presented.

O 27.8 Tue 11:30 H32

Doping of organic semiconductors in case of dopant precipitation: the internal interface charge transfer doping model — •Thomas Mayer[1,2], Eric Mankel[1,2], Corinna Hein[1], and Wolfram Jaegermann[1,2] — [1]Technische Universität Darmstadt, Institute of Materials Science, Surface Science Division — [2]Innovation Lab Heidelberg

Doping of organic semiconductors is of paramount interest for device optimization as in addition to improved conductivity, engineering of space charge regions at interfaces e.g. of donor acceptor heterojunction solar cells is achieved. Photoemission data taken at the synchrotron BESSY on co-sublimed and bilayer films of prototypical organic semiconductors as CuPc and spiro-MeoTAD and prototypical p-type organic and inorganic dopants as TCNQ and WO3 show similar electronic trends, which can be explained assuming phase separation of the dopants within the matrix material. For metal oxides the precipitation is directly observed using TEM. For the doping induced variations of the matrix Fermi level in such semiconductor-dopant composites we propose the internal interface charge transfer doping model. According to this model the doping limit can be predicted from pristine matrix and pristine dopant electronic band diagrams. The model also admits of deriving measures that can be taken to improve doping efficiency.

O 27.9 Tue 11:45 H32

Molecular orientation at heterojunctions for organic photovoltaics studied by NEXAFS — •Andreas Opitz[1], Norbert Koch[1], Ulrich Hörmann[2], Wolfgang Brütting[2], Christopher Lorch[3], Alexander Hinderhofer[3], Frank Schreiber[3], and Ellen Moons[4] — [1]Inst. f. Physik, Humboldt-Universität zu Berlin, Germany — [2]Inst. of Physics, University of Augsburg, Germany — [3]Inst. of Applied Physics, University of Tübingen, Germany — [4]Dept. of Physics and Electrical Engineering, Karlstad University, Sweden

Organic/organic heterojunctions are widely used in organic photovoltaic cells. The morphology at the interface, where the charge carrier separation takes place, plays an important role. In this contribution the interfaces between sexithiophene (6T) as donor and the acceptor materials fullerene (C$_{60}$) and diindenoperylene (DIP) [1] were analysed by angle resolved near-edge X-ray absorption fine structure spectroscopy and the results were compared to X-ray scattering data.

Different orientations are observed for molecules in the bulk, at free surfaces and at buried interfaces. Here, the orientation at the free surfaces depends on the substrate temperature during deposition for 6T but not for DIP. Furthermore, the acceptor molecules influence the orientation of the underlying 6T molecules. An improved crystallization and pronounced upright standing of the molecules in the underlying 6T film was observed upon deposition of C$_{60}$. In contrast the deposition of DIP on top of 6T leads to an orientational relaxation of the 6T molecules to the bulk inclination angle.

[1] U. Hörmann et al., phys. stat. sol. RRL 5 (2011) 241.

O 27.10 Tue 12:00 H32

Electronic interface properties of PCBM using photoelectron spectroscopy — •Julia Maibach[1,2], Eric Mankel[1,2], Thomas Mayer[1,2], and Wolfram Jaegermann[1,2] — [1]Technische Universität Darmstadt, Fachbereich Materialwissenschaft — [2]InnovationLab GmbH, Heidelberg

The electronic interface properties of wet processed organic materials are of current interest as many fabrication techniques for organic electronic devices are based on inks. Photoelectron spectroscopy (PES) has proven to be a powerful method to investigate the electronic structure at semiconductor contacts. Due to high surface sensitivity of PES, the interface is generally prepared step by step in UHV. For films deposited from solution we integrated a newly developed ultrasonic nebulizer unit to the UHV cluster-tool of the analytic competence center at the InnovationLab, Heidelberg. Dilute solutions of Phenyl-C61-butyric acid methyl ester (PCBM) in Chlorobenzene were used to deposit the material on ozone and polymer treated ITO as well as on gold to investigate the contact behavior of PCBM. With the nebulizer method layer thicknesses in the range of 10-20 Å can be achieved while repeated exposure to the nebulae increased step by step the emission intensities of the PCBM. Furthermore drop-casting of thicker layers has been performed allowing in combination the thickness dependent determination of the electronic properties. In case of PCBM on ozone treated ITO the HOMO spectra shift 0.4 eV to higher binding energy with increasing thickness, indicating the formation of a space charge region in PCBM due to electron transfer from ozone treated ITO.

O 27.11 Tue 12:15 H32

Carbon Nanotubes and Organic Solar Cells — •Gerhard Lackner[1], Richard Boucher[2], Vladimir Shvartsmann[1], Viktor Bezugly[2], Ingolf Endler[3], Mario Krug[3], Frank Meissner[3], Martin Mkandawire[4], and Doru C. Lupascu[1] — [1]Universität Duisburg-Essen, Essen, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Fraunhofer-Institut für Keramische Technologien und Systeme IKTS, Dresden, Germany — [4]Verschuren Centre for Sustainabilty in Energy and the Environment, Cape Breton University, Canada

Materials like carbon nanotubes (CNT) attracted much attention by researchers all around the world due to their exceptional electrical, mechanical and chemical properties. Especially single-walled carbon nanotubes (SW-CNT) offer great opportunities in the field of new electrical devices, for instance field effect transistors based on their semiconductor properties. CNT are also used in organic photovoltaics (OPV) as acceptor material, to enhance charge carrier transport within organic layers or as transparent electrodes. The application of CNT as acceptor material and for charge carrier enhancement is the main topic of this work. Therefore, we studied the photovoltaic device performance of different material combinations of CNT, regio regular Poly(3-Hexylthiophen-2,5-diyl) (rr-P3HT), Phenyl-C61-butric acid methyl ester (PCBM) and copper phthalocyanine (CuPc). Furthermore, different device architectures were investigated and compared with each other.

O 27.12 Tue 12:30 H32

n-channel percolation in a pentacene-C60 ambipolar or-

ganic thin film transistor — Simon Noever, Stefan Fischer, and •Bert Nickel — Ludwig-Maximilians-Universität, Fakultät für Physik & CENS, München, D

We present [1] a well balanced ambipolar organic field effect transistor with high hole and electron saturation mobilities of 0.28 cm*/Vs and 0.18 cm*/Vs, respectively. The structure and morphology of the respective films are analyzed using AFM and GIXS methods. Furthermore, we track the formation of a pentacene-C60 heterojunction by in-situ measurements during deposition of C60. Upon percolation of the n-channel, the heterojunction charges, acting as an additional top gate for the hole conducting channel. The fact that the p-channel threshold does not shift before the n-channel develops highlights two interesting findings for bilayer ambipolar TFTs. Apparently, before the C60 film percolates, the fullerene islands are electronically floating and the charging of the interface is confined to the pentacene-C60 contact area. Secondly, the threshold voltage shift of the p-channel upon fullerene percolation implicates the generation of a second hole conducting channel at the pentacene top surface. The introduced method demonstrates a way to evaluate the electrostatic situation in operating organic heterojunction devices. [1] S. Noever, S. Fischer, B. Nickel, Advanced Materials (in press)

O 28: Focussed Session: Frontiers of Electronic Structure Theory III (jointly with HL and TT)

Time: Tuesday 10:30–13:15 Location: H36

Topical Talk O 28.1 Tue 10:30 H36

Materials for Alternative Energies: Computational Materials Discovery and Crystal Structure Prediction — •Chris Wolverton — Northwestern University, Evanston, IL, USA

Many of the key technological problems associated with alternative energies may be traced back to the lack of suitable materials. The materials discovery process may be greatly aided by the use of computational methods, particular those atomistic methods based on density functional theory. In this talk, we present an overview of recent work on energy-related materials from density-functional based approaches. We have developed novel computational tools which enable accurate prediction of crystal structures for new materials (using both Monte Carlo and Genetic Algorithm based approaches), materials discovery via high-throughput, data mining techniques, and automated phase diagram calculations. We highlight applications in the area of Li battery materials and hydrogen storage materials.

O 28.2 Tue 11:00 H36

Doping at the Si-SiO2 interface — Fabiano Corsetti[1] and •Arash Mostofi[2] — [1]CIC nanoGUNE Consolider, Donostia-San Sebastian, Spain — [2]Dept. of Materials & the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, UK

The Si-SiO2 interface is a common feature in modern silicon-based CMOS technology for the fabrication of integrated circuits. The ongoing miniaturisation drive for such devices makes it increasingly important to understand the effect of the interface on the dopant distribution and properties. Indeed, in some cases channel lengths can be a few tens of nanometres, with the device properties being determined by only about 100 dopant atoms.

We have investigated the properties of arsenic dopants at the Si-SiO2 interface. We use a large supercell to simulate both ordered (α-cristobalite) and disordered silica interfaces with crystalline Si. The disordered interface is generated using a multiscale approach in which a Monte Carlo method, parametrised with density-functional theory (DFT) calculations, is used to access the long time scales required for amorphising the oxide. The segregation of arsenic dopants in silicon at the interface is then studied using DFT.

We are able to accurately characterise the long-range quantum confinement effect due to the interface, which is found to result in a small energy barrier for segregation. We also investigate the effect of the local stress at the defect site on its segregation energy, and show that a simple ‘particle in a box’ model can be used to explain the calculated segregation energies at all substitutional silicon sites.

O 28.3 Tue 11:15 H36

Pressure-induced structural transformations in nanomaterials: a linear-scaling DFT investigation — •Niccolo Corsini[1], Peter Haynes[1], Carla Molteni[2], and Nicholas Hine[1] — [1]Imperial College, London, UK — [2]King’s College, London, UK

Semiconductor nanomaterials, including nanocrystals, nanorods and tetrapods, display a number of peculiar and tunable properties that distinguish them from their bulk counterparts and make them versatile materials for use as e.g. effective optical probes in medical diagnostics or photovoltaic devices. Of particular interest is their response to applied pressure, as they transform from one crystalline or amorphous structure to another. Accurate simulations are important for understanding finite size effects in the atomistic mechanisms of phase transformations (difficult to observe clearly in macroscopic experiments), for the opportunity to uncover novel metastable phases stabilized in finite systems, and for potentially innovative applications of nanomaterials. First-principles methods are essential to accurately describe the bond breaking/making in phase transformations and the realistic description of surfaces (often covered by complex surfactants). However the computational cost limits both the length- and time-scales attainable. We have combined an order-N density functional theory code for large systems and an electronic-enthalpy method to apply pressure to finite systems to model with quantum mechanical precision processes induced by pressure in nanomaterials (including their surfaces) under realistic conditions. The focus is on Si, CdSe and CdS nanocrystals that are currently favoured for technological applications.

O 28.4 Tue 11:30 H36

Density functional / molecular dynamics simulations of nucleus-driven crystallization of amorphous Ge2Sb2Te5 — •Jaakko Akola[1,2,3], Janne Kalikka[4], Julen Larrucea[4], and Robert O. Jones[3] — [1]Department of Physics, Tampere University of Technology, Finland — [2]COMP Centre of Excellence, Department of Applied Physics, Aalto University, Finland — [3]GRSS and PGI-1, Forschungszentrum Jülich, Germany — [4]Nanoscience Center, Department of Physics, University of Jyväskylä, Finland

Early stages of nucleus-driven crystallization of the prototype phase change material Ge2Sb2Te5 have been studied by massively-parallel density functional/molecular dynamics simulations for amorphous samples (460 and 648 atoms) at 500, 600, and 700 K [1]. All systems assumed a fixed cubic seed of 58 atoms and 6 vacancies in order to achieve sub-nanosecond phase transition. Crystallization occurs within 600 ps for the 460-atom system at 600 and 700 K, and signs of crystallization (nucleus growth, percolation) are present in the others. Crystallization is accompanied by an increase in the number of ABAB squares (A: Ge, Sb, B: Te) [2,3], and atoms of all elements move significantly. The evolution of cavities/vacancies is closely monitored. The existence of Te-Te, Ge-Ge, Ge-Sb, and Sb-Sb (wrong) bonds is an inevitable consequence of rapid crystallization.

[1] J. Kalikka, J. Akola, J. Larrucea, and R. O. Jones, Physical Review B 86, 144113 (2012). [2] J. Akola and R. O. Jones, Phys. Rev. B 76, 235201 (2007). [3] J. Akola and R. O. Jones, Phys. Rev. Lett. 100, 205502 (2008).

O 28.5 Tue 11:45 H36

Large-Scale Moiré Patterns of hexagonal Boron Nitride on Cu(111): DFT Studies of Structural and Electronic Properties — •Ralph Koitz, Ari P Seitsonen, Marcella Iannuzzi, and Jürg Hutter — Institute of Physical Chemistry, University of Zurich, Switzerland

Hexagonal boron nitride (h-BN) adsorbed on metal surfaces shows great promise for applications in nanoscience. Interesting structural and electronic properties have been found, e.g. for h-BN on Rh(111) and Ru(0001), where the overlayer is strongly corrugated. Recent experiments with h-BN on Cu(111) indicate that the difference in lattice constants and a rotation of the monolayer lead to moiré patterns with periodicities greater than 5 nm. To thoroughly understand this system, however, further insight is needed at the atomic level.

In this contribution we present an in-depth DFT study of a moiré pattern of a rotated 24×24 h-BN sheet on a 23×23 Cu(111) slab. The periodic pattern extends over 6 nm, making this simulation the largest of its kind so far reported. We study the gradual change of adsorption registry of the monolayer, and its influence on the electronic structure.

Both B and N occupy the entire range of *top, hcp, fcc*, and bridging positions. This modulation over the unit cell is reflected in the projected DOS, the electrostatic potential, and the contrast in simulated STM images. Contrary to other *h*-BN/metal systems, only minute structural changes occur upon adsorption. Our results show that the observed corrugation is chiefly electronic in nature and strongly related to the lateral variation of adsorption registries.

O 28.6 Tue 12:00 H36

A computational perspective for the development of electronic excited-states calculations — •Xavier Andrade — Department of Chemistry and Chemical Biology, Harvard University, Cambridge, United States

In this talk I present different aspects of my work, focused on improving electronic structure theory for excited states with the aim of making it suitable for current computer architectures.

First, I will present an approach to approximate the exchange and correlation (XC) term in density functional theory. In this approach the XC potential is considered as an electrostatic potential. Based on this representation we develop a scheme that fixes the asymptotic behavior of an approximated XC potential. Additionally, from the procedure it is possible to extract the derivative discontinuity of the XC potential to directly obtain the gap of atoms and molecules.

Real-time methods like molecular dynamics and real-time time-dependent density functional theory are a good alternative for computing response properties. However, long propagation times are needed to obtain resolved properties. As a second topic of this talk, we address this problem by using a state-of-the-art signal-analysis technique: compressed sensing. By using this method instead of a Fourier transform, we find that the total propagation time required for resolved spectra can be reduced by a factor of five.

Finally, I will discuss my work on electronic structure calculations on graphical processing units (GPU) and the strategies to profit from the data parallelism available in the density functional formalism.

O 28.7 Tue 12:15 H36

Nuclear quantum effects in first principles molecular dynamics by colored-noise thermostats — •Michele Ceriotti — University of Oxford, United Kingdom

Oftentimes atomistic computer simulations treat atomic nuclei as purely classical particles, even when the electronic structure problem is treated quantum mechanically. This is a very good approximation when the system contains only heavy atoms. However, lighter nuclei such as hydrogen exhibit a strong quantum behavior, which manifests itself as sizable zero-point energy, tunnelling, isotope effects, etc.

Path integral methods are the state-of-the-art technique to model quantum nuclei, but they are computationally very demanding. Here I will discuss how a correlated-noise Langevin dynamics can be used to approximate nuclear quantum effects inexpensively, and how it can reduce by an order of magnitude the cost of quantitatively accurate path integral molecular dynamics. I will also present applications to the simulation of nuclear quantum effects in hydrogen-bonded materials by ab initio molecular dynamics.

O 28.8 Tue 12:30 H36

Semiconductor and Metal-Oxide Nanocrystal Simulations with Linear-Scaling PAW DFT — •Nicholas Hine — Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom — Cavendish Laboratory, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Nanocrystals enable tuning of material properties by varying attributes not available in bulk crystals, such as size, shape and surface termination, and such systems have innumerable applications in the field of energy materials, particularly in photovoltaics and photocatalysis. While whole nanocrystals are too large to be studied with traditional cubic-scaling first-principles methods, linear-scaling formulations of density functional theory (LS-DFT) enable the study of systems of many thousands of atoms. This allows nanocrystal simulations to make contact with the realistic size regime of 5-10nm, thus overlapping with the feasible scale of experimental characterisation and control. I will discuss recent developments in the ONETEP LS-DFT code that enable these large-scale, high-accuracy simulations, including the Projector Augmented Wave method, and recent applications to TiO2 nanocrystals, pressure-induced phase transformations in II-VI semiconductor nanocrystals, and wurtzite-structure III-V semiconductor nanorods. I will discuss the origin of the large dipole moments which can be observed in such structures, and show how an effect akin to Fermi-level pinning can have a determining influence on the overall polarisation, explaining its variation with size, shape, surface chemistry and composition.

O 28.9 Tue 12:45 H36

Many-body effects on the carrier dynamics of graphene — •Cheol Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul, Korea

It is very important to understand how a charge carrier in real materials interacts with other charge carriers or with the lattice vibration. In this presentation, I will explain that the measured carrier scattering rate versus energy behavior in graphene can be quantitatively described from first-principles calculations considering electron-electron interactions within the GW approximation and electron-phonon interactions within the Migdal approximation [1]. Then, I will show that our calculation can also explain (i) the mismatch between the extrapolations of the upper and lower Dirac cones in heavily doped graphene [2] and (ii) the significant deviation from linear energy dispersion in extremely low-doped graphene [3]. Last, I will show that first-principles calculations on the intrinsic electrical resistivity of graphene arising from electron-phonon interactions [4] can quantitatively explain the transport experiments on heavily doped graphene [5].

[1] C.-H. Park, F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. 99, 086804 (2007).

[2] C.-H. Park, F. Giustino, C. D. Spataru, M. L. Cohen, and S. G. Louie, Nano Lett. 9, 4234 (2009).

[3] D. A. Siegel, C.-H. Park, C. Hwang, J. Deslippe, A. V. Fedorov, S. G. Louie, and A. Lanzara, Proc. Nat. Acad. Sci. 108, 11365 (2011).

[4] C.-H. Park et al., in preparation.

[5] D. K. Efetov and P. Kim, Phys. Rev. Lett. 105, 256805 (2010).

O 28.10 Tue 13:00 H36

Theory of nanomagnetic and graphene hybrid systems: adatoms and multiorbital Kondo physics — •Tim Wehling — Institute for Theoretical Physics and BCCMS, University of Bremen, D-28359 Bremen, Germany

Graphene combines chemical inertness with a distinctly symmetric low energy electronic structure. Here, we show based on first-principles calculations that these two characteristics largely determine its interaction with adatoms. We find that covalent bonds to first row elements cause midgap states which can control electron transport [1] and the dielectric properties [2] of graphene based systems. The special nature of the Dirac electrons furthermore governs the coupling of magnetic adatoms to graphene by orbital selection rules and leads to peculiar multiorbital Kondo physics [3,4]. Finally, it is shown how multiorbital effects control the physics of magnetic transition metal atoms coupled to normal metals [5] and topological insulators [6].

[1] T. O. Wehling et al., Phys. Rev. Lett. 105, 056802 (2010).
[2] S. Yuan et al., Phys. Rev. Lett. 109, 156601 (2012).
[3] T. O. Wehling et al., Phys. Rev. B 84, 235110 (2011).
[4] T. O. Wehling et al., Phys. Rev. B 81, 115427 (2010).
[5] B. Surer et al., Phys. Rev. B 85, 085114 (2012).
[6] J. Honolka et al., Phys. Rev. Lett. 108, 256811 (2012).

O 29: Organic/bio Molecules on Metal Surfaces III

Time: Tuesday 10:30–13:15 Location: H38

O 29.1 Tue 10:30 H38

Optically and thermally induced reactions of an azobenzene derivative on Bi(111) — •Christopher Bronner[1], Beate Priewisch[2], Karola Rück-Braun[2], and Petra Tegeder[1,3] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [2]Technische Universität Berlin, Institut für Chemie, Straße des 17. Juni 115, 10623 Berlin, Germany — [3]Ruprecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

Molecular switches which undergo photo-induced isomerization reactions are considered promising building blocks in the development of nanotechnological devices such as data storage, molecular electronics or functionalized surfaces. Generally, such systems are envisioned to be mounted at surfaces or interfaces of solids. However, the majority of such molecules lose their switching functionality when adsorbed directly on a (metal) surface, which is usually attributed to electronic coupling and/or steric hindrance. Controlled tuning of the coupling strength in these adsorbate/substrate systems is therefore considered crucial to restore functionality.

We found that di-meta-cyano-azobenzene (DMC) adsorbed on a semi-metallic bismuth substrate undergoes a photo-induced trans-cis isomerization reaction both in the first layer and the multilayer, while the photo-induced back-reaction is not observed. In addition, we found a thermally activated reaction of the cis isomer.

O 29.2 Tue 10:45 H38

The effect of molecular coverage and molecular vibrations on the adsorption geometry of azobenzene on Ag(111) — •Giuseppe Mercurio[1,2], Reinhard Maurer[3], Wei Liu[4], Sebastian Hagen[5], Felix Leyssner[5], Jörg Meyer[3], Alexandre Tkatchenko[4], Petra Tegeder[5], Sergey Soubatch[1,2], Karsten Reuter[3], and Frank Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology — [3]Department Chemie, TU München, Germany — [4]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [5]Freie Universität Berlin, Fachbereich Physik, Berlin, Germany

Experimentally determined adsorption geometries of molecular switches are essential both for understanding their functionality and for benchmarking ab initio calculations. We investigate a prototypical molecular switch, i.e. azobenzene (AB), on the Ag(111) surface by means of the normal incidence x-ray standing wave (NIXSW) technique and dispersion-corrected density-functional theory (DFT) calculations. We find that the inclusion of non-local many-body screening in the $\text{DFT+vdW}^{\text{surf}}$ scheme [1] improves the description of AB. Coverage-dependent calculations reveal the most stable AB packing on Ag(111). The best agreement with NIXSW data is obtained if the additional effect of molecular anharmonic vibrations on the energetically most favorable AB adsorption geometry is taken into account.

[1] V. Ruiz et al. Phys. Rev. Lett. 108, 146103 (2012).

O 29.3 Tue 11:00 H38

Computationally efficient excited state properties of hybrid organic/inorganic systems: dynamics and spectroscopy with Delta Self-Consistent-Field Density Functional Theory (ΔSCF-DFT) — •Reinhard J. Maurer and Karsten Reuter — Technische Universität München, Lichtenbergstrasse 4, 85748 Garching, Germany

Understanding photon- or electron-induced changes in functional molecules adsorbed on well defined substrates forms the basis for rational molecular device design. Predictive-quality *ab initio* modelling of such surface-mounted devices has to be able to supply spectroscopic properties, not just accurately, but also in a computationally efficient manner. Current methods lack either the one or the other property. In this context, we present an approach further extending recent developments in Δ-Self-Consistent-Field Density-Functional-Theory (ΔSCF-DFT) [1].

We illustrate the rationale behind our approach and its performance for organic molecules adsorbed at metal surfaces. The method yields a topologically correct description of excited state potential energy surfaces and an accurate simulation of spectroscopic properties, such as photoemission or photoadsorption. Although a prior knowledge of the corresponding gas-phase properties of the adsorbate and cautious benchmarking are prerequisites to reliable results, the method can be readily applied to a variety of systems. [1] Gavnholt *et. al.*, PRB **78**, 075441 (2008).

O 29.4 Tue 11:15 H38

Dynamics of charging and bond formation of adsorbates on an ultrathin, insulating film supported by a metal substrate: A density functional study based on the perfect conductor model — •Ivan Scivetti and Mats Persson — Surface Science Research Centre, the University of Liverpool, Liverpool L69 3BX, UK

The ability to characterise and manipulate single atoms and molecules on ultrathin, insulating films by scanning tunnelling probe techniques has opened up a new frontier in atomic scale science. A most interesting aspect of these systems is the decoupling of the electronic states of the adsorbates from the metal substrate, which still allows for characterisation and manipulation by tunnelling electrons.

The description of the electronic and geometric structure and the dynamics of these systems exhibiting multiple charge states is very challenging for theory. Density Functional Theory (DFT) calculations are in many cases prohibitive because of the size of these systems and the delocalization error in current exchange-correlation functionals. In this work, we present a new simplified DFT scheme in which the metallic support is replaced by a perfect conductor. This scheme circumvents the limitations of standard DFT and allows us to treat various charge states of adsorbates, together with a considerable reduction of the computational effort. In particular, we are able to carry out ab-initio molecular dynamics on an excited (charged) state potential energy surface. We will show some interesting applications of this scheme to different charge states of metal adatoms and the dynamics of reversible bond formation in a metallo-organic molecule.

O 29.5 Tue 11:30 H38

Energetics of azobenzenes on noble metal surfaces — •Michael Schulze[1], Reinhard Maurer[2], Christopher Bronner[1], Karsten Reuter[2], and Petra Tegeder[1,3] — [1]Freie Universität Berlin, Fachbereich Physik — [2]TU München, Theoretische Chemie — [3]Ruprecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut

Temperature programmed desorption measurements and density-functional theory (DFT) calculations have been employed, to investigate the adsorption properties, in particular the binding energies, of azobenzenes on noble metal surfaces. The studied systems are the unsubstituted azobenzene and tetra-tert-butyl-azobenzene (TBA) on Au(111) and Ag(111), respectively. The only photoisomerizing system out of the four, TBA/Au(111), has been found to be the one with the strongest binding energy. These findings are explained by the larger bending angle of the molecule and the energetic overlap and hence a hybridization of the highest occupied molecular orbital (HOMO) of TBA with the Au(111) d-bands, which has also been proposed in order to elucidate the excitation mechanism in the photoisomerization [1].

[1] Ch.Bronner, M. Schulze et al 2012 New J. Phys. 14 043023

O 29.6 Tue 11:45 H38

Photo-switching of diluted azobenzene-based SAMs on Au(111) — •Thomas Moldt[1], Daniel Brete[1], Daniel Przyrembel[1], Joel R. Goldman[2], Rafal Klajn[2], Cornelius Gahl[1], and Martin Weinelt[1] — [1]Freie Universität Berlin, Department of Physics, Arnimallee 14, 14195 Berlin — [2]Weizmann Institute of Science, Department of Organic Chemistry, 76100 Rehovot, Israel

Photoisomerization of azobenzene within densely packed self-assembled monolayers (SAMs) of azobenzene-terminated alkanethiols is strongly suppressed.[1,2]. This is attributed to steric hindering [2] and/or excitonic coupling [3] among the chromophores. In this work we examine SAMs of 11-[(4-phenylazo)phenoxy]-undecane-1-thiol diluted with dodecane-1-thiol prepared by co-adsorption from solution. By differential reflectance spectroscopy (DRS) we demonstrate that the molecules self-assemble at the Au(111) surface whereby the azobenzene concentration is adjustable through the relative concentrations in solution. The azobenzene chromophores form aggregates with the excitonic shift of the S_2 absorption band decreasing with dilution. In addition near-edge X-ray absorption fine structure spectroscopy (NEXAFS) reveals changes of the orientation of the azobenzene photoswitch in the pure and mixed SAMs. In contrast to the pure azobenzene SAM, the mixed SAMs can be optically switched with high quantum efficiency.

[1] Evans et al., *Langmuir*, 1998, **14**, 6436-6440
[2] Wang et al., *J. Electroanal. Chem.*, 1997, **438**, 213-219
[3] Gahl et al., *J. Am. Chem. Soc.*, 2010, **132**, 1831-1838

O 29.7 Tue 12:00 H38

On-Surface Polymerization of 1,4-Diethynylbenzene on Cu(111) — •Johanna Eichhorn[1,2], Wolfgang M. Heckl[1,2], and Markus Lackinger[1,2] — [1]Department of Physics & TUM School of Education, Tech. Univ. Munich, 80799 Munich, Germany — [2]Deutsches Museum, 80538 Munich, Germany

The last decade has witnessed a growing interest in the use of organic materials in light-emitting diodes, and optoelectronic devices. In this context, the conjugated polymer poly(phenylene butadiynylene) has shown promising properties like photo-, and electroluminescence.[1] A previous study already reported that 1,4-diethynylbenzene (DEB) can be polymerized into PPB strands within Cu2+ functionalized mesoporous materials.[2] For a more facile preparation, we study polymerization of DEB on catalytically active Cu(111) surfaces by means of ultra-high vacuum scanning tunneling microscopy.

Upon adsorption at room temperature, DEB self-assembles into a densely packed structure controlled by weak hydrogen bonds (C-H...triple bond). Subsequent thermal annealing results in drastic structural changes, where wormlike chains containing Y-shaped trimers, cross-linked tetramers and dumbbell shaped hexamers were observed. The thermal stability of these surface-supported structures extends up to 450°C, thereby proofing covalent bond formation. The observed topology of the covalent networks can only be explained by at least two different coupling schemes: di- and trimerization.

[1] X. Zhan, et al., Adv. Mater., 2000, 12, 51-53.

[2] V. S.-Y. Lin, et al., J. Am. Chem. Soc., 2002, 124, 9040-9041.

O 29.8 Tue 12:15 H38

From physisorption to chemisorption: tuning the interaction of cyclooctatetraene with noble metal surfaces — •Martin Callsen[1], Hasmik Harutyunyan[2], Tobias Allmers[2], Nicolae Atodiresei[1], Vasile Caciuc[1], Daniel Wegner[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Physikalisches Institut and Center for Nanotechnology (CeNTech) Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Embedding specifically designed organic molecules into molecular devices or connecting them to an electronic circuit is a technological relevant aspect of molecular electronics. Recently designing molecular switches as one class of possible applications either by redox reactions or by conformational changes has been pursued. In a combined STM and DFT study we have investigated cyclooctatetraene (COT) adsorbed on different noble metal substrates as a possible candidate for a conformational switch. The role of charged states which change the conformation of COT in the gas phase is taken by the different strength of hybridization between the COT molecule and the surface. Long range dispersion interactions have been taken into account via a semi-empirical approach [1] and the non-local xc-functional vdW-DF [2] as implemented in a recent version of the JuNoLo code [3].

[1] S. Grimme *et al.*, J. Chem. Phys. **132**, 154104 (2010)

[2] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004)

[3] M. Callsen *et al.*, Phys. Rev. B **86**, 085439 (2012)

O 29.9 Tue 12:30 H38

Adsorption of V-TCNE on Ag(001): results from ab-initio calculations — •Thorsten Deilmann, Peter Krüger und Michael Rohlfing — Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany

Organic molecules coupled to transition metal atoms offer interesting physical properties like large magnetic moments. Recently, Wegner et al. [1] have shown that tetracyanoethylen (TCNE) and vanadium on Ag(001) can be induced by STM manipulation to form a strong chemical bond. Here, we present a theoretical study on the adsorption of V-TCNE on Ag(001). Optimized structures, adsorption energies, electronic and magnetic properties have been calculated employing density-functional theory. TCNE adsorbs in *on top* position with the nitrogen atoms bound to Ag surface atoms. Due to the interaction with the surface, an electron transfer occurs and the molecule is negatively charged. The calculated density of states, as well as the simulated STS and STM images show good agreement with respective experimental data [1].

Addition of vanadium leads to a spin-polarized system. We find that V atoms adsorb only at the *hollow* position on Ag(001). In the energetically most favored structure of V-TCNE, two nitrogen atoms are bound to a vanadium atom. Close to the Fermi level, the local density of states shows a dominant V induced peak that is distinctly broadened due to the molecule-substrate interaction.

[1] D. Wegner et al., *Phys. Rev. Lett.* **103**, 087205 (2009)

O 29.10 Tue 12:45 H38

Trimesic acid-assisted self-assembly of oligoethynylene-thiophene macrocycles: A donor-acceptor rectifier bilayer — •Jose D. Cojal[1], Masahiko Iyoda[2], and Jürgen P. Rabe[1] — [1]Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Department of Chemistry, Tokyo Metropolitan University, Tokyo, Japan

Fully conjugated π-expanded macrocyclic oligothiophenes [1] have attracted considerable interest due to their structural and optoelectronic properties. They have been envisaged for photovoltaic applications, host-guest systems and as building blocks of supramolecular nanostructures. Here, a self-assembled monolayer of trimesic acid (TMA) at the interface between its heptanoic acid solution and highly oriented pyrolytic graphite (HOPG) provided a way to template the 2D self-assembly of oligoethynylene-thiophene macrocycles. The so-formed bilayer was confirmed using STM tomography [2], i.e. discrete bias set-point imaging of each layer. Scanning Tunneling Spectroscopy of the macrocycle layer allowed us to determine the HOMO-LUMO gap of the bilayer and the position of the combined frontier orbitals, The I-V characteristics revealed an underneath TMA layer with acceptor (A) characteristics and an upper donor (D) macrocycle layer, forming a D-A rectifier bilayer.

[1] K. Nakao, M. Nishimura, T. Tamachi, Y. Kuwatani, H. Miyasaka, T. Nishinaga and M. Iyoda, J. Am. Chem. Soc. 128 (2006) 16740

[2] C. Seifert, D. Skuridina, X. Dou, K. Müllen, N. Severin and J. P. Rabe, Phys. Rev. B 80 (2009) 245429

O 29.11 Tue 13:00 H38

Investigation of Mn_{12} single molecule magnets on surfaces deposited by means of electrospray ionization — •Philipp Erler[1], Stefan Ambrus[2], Sebastian Höll[1], Samuel Bouvron[1], Ulrich Groth[2], Elizabeta Cavar[1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]Fachbereich Chemie, Universität Konstanz, 78457 Konstanz

Single molecule magnets (SMMs), like Mn_{12}-acetate, have attracted significant interest during the past decades due to their unique magnetic properties like hysteresis of pure molecular origin and the possibility to observe quantum tunneling of magnetization. This material class allows for basic studies on quantum effects of magnetism on the molecular scale and is furthermore a promising candidate for preliminary studies aiming at ultrahigh density data storage devices or quantum computing applications. However, progress in this field is hindered by the difficulty of depositing intact SMMs on surfaces.

Here we present a study of Mn_{12}-acetate molecules deposited on different noble metal surfaces by means of electrospray ionization in ultra high vacuum. In contrast to wet chemical preparation procedures, this method offers the advantages of a high sample quality, full control over the surface coverage and a free choice of the substrate and the molecular ligand shell. We studied the structural and electronic properties of sub-monolayers of Mn_{12} molecules using low temperature scanning tunneling microscopy and spectroscopy (STM/STS). Molecular islands, chain like structures as well as individual clusters were investigated.

O 30: Plasmonics and Nanooptics III

Time: Tuesday 10:30–13:00 Location: H31

O 30.1 Tue 10:30 H31

Time-resolved wave packet observation of surface plasmon polaritons provided by normal incidence photoemission electron microscopy — •Philip Kahl[1], Simon Sindermann[1], Christian Schneider[2], Alexander Fischer[2], Martin Aeschlimann[2], Michael Horn-von Hoegen[1], and Frank-J. Meyer zu Heringdorf[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, 47057 Duisburg — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern

In order to observe surface plasmon polaritons (SPPs) in a photoemission electron microscopy (PEEM) experiment, ultrashort (sub 20 fs) laserpulses of 800 nm wavelength are directed onto a surface with plasmonic Ag or Au nanostructures. In the past, non-linear photoemission under grazing incidence was used to obtain a Moiré type contrast of propagating SPPs waves. The possibility of a light incidence normal to the surface of the sample features the prospect of a direct observation of SPP wave fronts as the observed fringes resemble the SPP wavelength. This enables us to track a surface plasmon wave packet propagating at a metal-vacuum interface directly by using phase stabilized, time-resolved experiments under normal incidence conditions. Additionally, the SPP propagation parameters like group and phase velocity as well as the propagation length are measured.

O 30.2 Tue 10:45 H31

Coupled plasmonic waveguide arrays — •Alexander Block, Felix Bleckmann, and Stefan Linden — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn

Surface plasmon polaritons (SPPs) are hybrid electromagnetic waves propagating along a metal-dielectric interface. Their effective refractive index can be controlled by adding an additional dielectric on top of the metal. Varying the thickness of the dielectric layer allows us to fabricate structures with complex refractive index profiles. Here, we use negative-tone gray-scale electron beam lithography to define waveguide arrays made of PMMA on top of a gold film.

In our experiment SPPs are excited by focusing laser light onto a grating coupler and the resulting SPP propagation can be visualized by imaging the leakage radiation with a high numerical aperture objective. In contrast to other studies on coupled waveguide arrays our setup can directly observe the field intensities inside the waveguides. The results clearly show the coupling between the waveguides as predicted by the coupled mode theory. The coupling constant can be obtained as a function of the waveguides' thickness and their separation. These results agree well with finite element simulations which are also presented.

O 30.3 Tue 11:00 H31

Manipulation of Airy surface plasmon beams — •Felix Bleckmann[1], Alexander Minovich[2], Jakob Frohnhaus[1], Dragomir N. Neshev[2], and Stefan Linden[1] — [1]Physikalisches Institut, Universität Bonn, Nuasslle 12, 53115 Bonn, Germany — [2]Nonlinear Physics Centre and Centre for Ultrahigh-bandwidth Devices for Optical Systems (CUDOS), Research School of Physics and Engineering, The Australian National University, ACT 0200, Canberra, Australia

Airy plasmons are electromagnetic waves propagating at the interface of a metal and an insulator. In contrast to Gaussian shaped surface plasmons, Airy plasmons are diffractive-free and offer a self-healing behavior. We demonstrate that the propagation of Airy plasmons can be manipulated by adding a supplemental dielectric on top of the metal. More specifically, with controlled variation of the dielectric height a linear gradient of the effective index is producible. The trajectory of Airy plasmons can be controlled this way while preserving their unique non-diffractive properties.

Here, we use negative-tone grey-scale electron beam lithography to fabricate these GRIN plasmonic structures made of PMMA on top of a gold film. The bending of Airy surface plasmons due to the gradient of the effective refractive index is observed by leakage radiation microscopy. Our experimental results are in good agreement with numerical calculations.

O 30.4 Tue 11:15 H31

Morphological tuning of the plasmon dispersion in dielectric-loaded nanofiber waveguides — •Till Leissner[1], Christoph Lemke[1], Jacek Fiutowski[2], Jörn Radke[2], Alwin Klick[1], Luciana Tavares[2], Jakob Kjelstrup-Hansen[2], Horst-Günter Rubahn[2], and Michael Bauer[1] — [1]Christian-Albrechts-Universität zu Kiel, IEAP, 24098 Kiel (Germany) — [2]Mads Clausen Institute, NanoSYD, University of Southern Denmark, Alsion 2, DK-6400 Sønderborg (Denmark)

Understanding the impact of lateral mode confinement in plasmonic waveguides is of fundamental interest regarding potential applications in plasmonic devices. The knowledge of the frequency-wave vector dispersion relation provides the full information on electro-magnetic field propagation in a waveguide. Here two-photon photoemission electron microscopy is used to measure the real part of the surface plasmon polariton dispersion relation in the near infrared spectral regime for individual nanoscale plasmonic waveguides, which were formed by deposition of para-Hexaphenylene (p-6P) based nanofibers on top of a gold film. Characterization by means of scanning electron microscopy and atomic force microscopy provides accurate information on the dimensions of the investigated waveguides and enables us to quantify the effect of mode confinement by comparison with experimental results from continuous p-6P films on a gold substrate and calculations based on the effective index method. Our results show that the structural control of the cross-sectional dimension of a p-6P nanofiber provides a promising means for the customized design of plasmonic waveguides.

O 30.5 Tue 11:30 H31

Propagating and localized surface plasmons probed in a counter-propagating photoemission electron microscopy detection scheme — •Christoph Lemke[1], Till Leissner[1], Alwin Klick[1], Jörn Radke[1], Stephan Jauernik[1], Jacek Fiutowski[2], Jakob Kjelstrup-Hansen[2], Horst-Günter Rubahn[2], and Michael Bauer[1] — [1]Institute for Experimental and Applied Physics, University of Kiel, D-24118 Kiel — [2]Mads Clausen Institute, University of Southern Denmark, DK-6400 Sønderborg

In an interferometric time-resolved photoemission electron microscopy (ITR-PEEM) experiment, the near-field associated with propagating surface plasmon polaritons (SPP) can be locally sensed via interference with ultrashort laser pulses. In this talk, we present ITR-PEEM data of SPP propagation at a gold vacuum interface recorded in a counter-propagating pump-probe geometry. In comparison to former work this approach provides a considerably improved access to the propagation and interaction dynamics of SPP wave packets. The potential of the scheme will be illustrated by two examples: In a first experiment we monitor the propagation of a SPP wave packet along a gold vacuum interface and extract in a rather direct manner characteristic parameters such as phase and group velocity. In a further example the counter-propagating ITR-PEEM scheme is used to investigate the excitation of localized surface plasmons at defined gold nanodots via propagating SPP wave packets. The experiments enable us to directly monitor in detail the interaction dynamics between these two collective modes in time and space.

O 30.6 Tue 11:45 H31

Infrared spectroscopy of single surface phonon polariton resonators — •Tao Wang, Benedikt Hauer, Peining Li, and Thomas Taubner — 1st Institute of Physics (1A), RWTH Aachen University, 52056, Aachen, Germany

Infrared spectroscopy is widely used to identify and characterize molecules. Recently, the sensitivity of infrared absorption spectroscopy was enhanced by several orders of magnitude with metallic optical antennas on dielectric substrates [1-2]. However, phonon-resonant nanostructures promise an even higher field enhancement compared to infrared metallic antennas [3].

In this work, we experimentally investigate the infrared spectroscopy of single surface phonon polariton (SPhP) resonators. The SPhP resonators are individual micro-size holes in a thin gold film fabricated by nanosphere lithography, which is deposited on a SiC substrate. The SPhP resonance of the single holes can be clearly seen from far-field extinction spectra and from near-field optical images. The strong field enhancement combined with the easy fabrication makes single SPhP resonators as a promising candidate for highly sensitive surface enhanced infrared absorption spectroscopy.

[1] R. Adato et al.; PNAS, 106, 19227 (2009)
[2] F. Neubrech et al.; PRL 101, 157403 (2008)
[3] R. Hillenbrand et al., Nature, 418, 159-162 (2002)

O 30.7 Tue 12:00 H31

Magnetic Circular Dichroism PEEM for the study of subwavelength all-optical magnetization switching in TbCo alloys — •Pascal Melchior[1], Markus Rollinger[1], Philip Thielen[1,3], Sabine Alebrand[1], Ute Bierbrauer[1], Christian Schneider[1], Stéphan Mangin[2], Mirko Cinchetti[1], and Martin Aeschlimann[1] — [1]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, Germany — [2]Institut Jean Lamour, Université de Lorraine, France — [3]Graduate School Materials Science in Mainz, Germany

Magnetization reversal using femtosecond laser pulses is a way to control magnetization without any external magnetic field. Combined with plasmonic antenna structures to focus light below the diffraction limit, plasmon-assisted laser-induced magnetization switching has the potential to revolutionize magnetic data storage. In order to study this phenomenon, an experimental method is needed that provides access to both magnetic as well as near-field properties. We show that photoemission electron microscopy (PEEM) combined with magnetic circular dichroism in the two-photon photoemission has the potential to fulfill this role. In particular, we show that high-anisotropy TbCo alloys, which are known to enable optical control over the magnetization, show a decent dichroic contrast in two-photon photoemission

PEEM enabling the imaging of magnetic domains. Furthermore, the possibility of plasmon-assisted magnetization switching on structured TbCo films will be discussed.

O 30.8 Tue 12:15 H31

Coherent two-dimensional nanoscopy of nanotextured thin-film Si solar cells — Martin Aeschlimann[1], Tobias Brixner[2], Matthias Hensen[3], •Christian Kramer[2], Pascal Melchior[1], Walter Pfeiffer[3], Martin Piecuch[1], Helmut Stiebig[4], Christian Strüber[3], and Philip Thielen[1] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [4]Malibu GmbH & Co.KG, Böttcher Str.7, 33609 Bielefeld

The absorption of thin-film solar cells can be enhanced by increasing the effective light path in the absorptive layer via light trapping. We investigated amorphous thin-film Si solar cells with nanotextured internal interfaces by using coherent 2D nanoscopy. This technique combines coherent 2D spectroscopy with photoemission electron microscopy and enables a high spatial resolution below the optical diffraction limit. In our experiments we observed hot-spot photoemission from the Si layer and found line-shape variations of local 2D nanospectra obtained from different spots on the Si surface. These results are consistent with the formation of localized modes of multiply scattered radiation that are responsible for an increased absorption in the Si layer. Furthermore, we fit the measured 2D nanospectra with a damped Lorentzian-oscillator model and received the spatially-resolved information about lifetimes and spectral shifts of localized photonic modes.

O 30.9 Tue 12:30 H31

Real-time observation of ultrafast Rabi oscillations between excitons and plasmons in J-aggregate/metal hybrid nanostructures — Parinda Vasa[1,2], Wei Wang[1], •Ephraim Sommer[1], Melanie Lammers[1], Margherita Maiuri[3], Cristian Manzoni[3], Giulio Cerullo[3], and Christoph Lienau[1] — [1]Institut für Physik and Center of Interface Science, Carl von Ossietzky Universität, 26129 Oldenburg, Germany — [2]Department of Physics, Indian Institute of Technology Bombay, 400076 Mumbai, India — [3]IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Milano, Italy

Surface plasmon polaritons (SPPs), optical excitations at the interface between a metal and a dielectric, carry significant potential for guiding and manipulating light on the nanoscale. Their weak optical nonlinearities, however, hinder active device fabrication, e.g., for all-optical switching or information processing. Recently, strong optical dipole coupling between SPPs and nonlinear quantum emitters with normal mode splittings of up to 700 meV has been demonstrated. The predicted ultrafast energy transfer between quantum emitters and SPP fields could be a crucial microscopic mechanism for switching light by light on the nanoscale. Here, we present the first real-time observation of ultrafast Rabi oscillations in a J-aggregate/metal nanostructure, evidencing coherent energy transfer between excitonic quantum emitters and SPP fields. We demonstrate coherent manipulation of the coupling energy by controlling the exciton density on a 10-fs timescale, a step forward towards coherent, all-optical ultrafast plasmonic circuits and devices.

O 30.10 Tue 12:45 H31

Collective spontaneous emission of strongly coupled exciton-surface plasmon polaritons — •Wei Wang[1], Parinda Vasa[1,2], Robert Pomraenke[1], Ralf Vogelgesang[1], Margherita Maiuri[3], Cristian Manzoni[3], Giulio Cerullo[3], and Christoph Lienau[1] — [1]Institut für Physik and Center of Interface Science, Carl von Ossietzky Universität — [2]Department of Physics, Indian Institute of Technology Bombay, 400076 Mumbai, India — [3]IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Milano, Italy

We report on the observation of collective spontaneous emission of strongly coupled excitons (Xs) and surface plasmon polaritons (SPPs) in J-aggregate/metal hybrid nanostructures. The optical response of the system is probed at the field level by angle-resolved spectral interferometry. We find that the strong coupling results in a pronounced modification of the radiative damping due to formation of super- and sub-radiant polariton states. Their ultrafast emission dynamics is measured in real time and is well explained within a coupled oscillator model. Such a strong modification of the radiative damping can open up new directions in coherent active plasmonics.

O 31: Surface and Interface Magnetism I (jointly with MA)

Time: Tuesday 10:30–13:15 Location: H33

O 31.1 Tue 10:30 H33

Magnetism of Fe on Pt(111) Revisited by Inelastic Scanning Tunneling Spectroscopy — Tobias Schlenk, Alexander Ako Khajetoorians, •Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, Hamburg University, Germany

We revisited the magnetism of single Fe atoms [1] and Fe-H_n complexes adsorbed on the surface of Pt(111) by means of magnetic field dependent inelastic scanning tunneling spectroscopy [2,3]. We found that the magnetic easy axis is either perpendicular to or within the surface plane, depending on an fcc or hcp adsorption site. Adsorption of H atoms changes the strength of the magnetic anisotropy and leads to Kondo screening for one of the two Fe-H_2 complexes. For all investigated cases, the magnetic anisotropy energy is almost an order of magnitude lower than recently reported [1].

[1] T. Balashov *et al.*, Phys. Rev. Lett. **102**, 257203 (2009).

[2] A. A. Khajetoorians, S. Lounis, B. Chilian, A. T. Costa, L. Zhou, D. L. Mills, J. Wiebe, and R. Wiesendanger, Phys. Rev. Lett. **106**, 037205 (2011).

[3] B. Chilian, A. A. Khajetoorians, S. Lounis, A. T. Costa, D. L. Mills, J. Wiebe, and R. Wiesendanger, Phys. Rev. B **84**, 212401 (2011).

O 31.2 Tue 10:45 H33

Structure Driven Complex Magnetic Ordering of a CoO Overlayer on Ir(100) — •Florian Mittendorfer[1], Josef Redinger[1], Raimund Podloucky[2], and Michael Weinert[3] — [1]Inst. of Applied Physics, TU Vienna — [2]Inst. of Physical Chemistry, Univ. Vienna — [3]Univ. Wisconsin-Milwaukee

The adsorption of a mono-layer thick magnetic oxide film on an unmagnetic substrate offers a playground to study the relation between the geometrical structure and the magnetic properties of the film.

I will present our recent results on the magnetic ordering in the ultrathin hexagonal c(10x2) CoO(111) film supported on Ir(100) [1], obtained on the basis of ab initio calculations with the Vienna Ab-initio Simulations Package (VASP). We find a close relationship between the local structural properties of the oxide film and the induced magnetic order, leading to alternating ferromagnetically and antiferromagnetically ordered segments. While the local magnetic order is directly related to the geometric position of the Co atoms, the mismatch between the CoO film and the Ir substrate leads to a complex long-range order of the oxide.

[1] Phys. Rev. Lett. 109 (2012) 015501.

O 31.3 Tue 11:00 H33

Detecting and Interpreting Spin-Dependent Dissipation Observed with Magnetic Exchange Force Microscopy and Spectroscopy — •Alexander Schwarz, Rene Schmidt, Elena Y. Vedmedenko, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

Magnetic exchange force microscopy (MExFM) and spectroscopy (MExFS) can resolve magnetic surfaces and probe the distance dependence of the magnetic exchange interaction with atomic resolution [1,2]. In both cases the frequency shift of an oscillating cantilever due to conservative tip-sample interactions is detected. By recording the amplitude and the excitation amplitude required to keep the amplitude of the cantilever oscillation constant, the energy loss due to dissipative processes can be determined. It turns out, that this signal can be spin-dependent as well [2,3]. The possible origin of this signal will be discussed in terms of spin-excitations [4] and spin-dependent adhesion-hysteresis [3]. Additionally, it will be shown how the dissipation signal can be used to characterize the tip, which is very important to correctly evaluate force spectroscopy data quantitatively.

[1] U. Kaiser, A. Schwarz and R. Wiesendanger, Nature 446, 522 (2007).

[2] R. Schmidt, A. Schwarz, and R. Wiesendanger, Phys. Rev. Lett. 106, 257202 (2011).

[3] E. Y. Vedmedenko et al., Phys. Rev. B 85, 174410 (2012).

[4] F. Pellegrini, G. E. Santoro, and E. Tosatti, Phys. Rev. Lett. 105, 146103 (2010).

O 31.4 Tue 11:15 H33

Zeeman splitting in superconducting scanning tunneling microscopy tips — •Matthias Eltschka[1], Berthold Jäck[1], Maximilian Assig[1], Markus Etzkorn[1], Christian R. Ast[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Scanning tunneling microscopy (STM) is a powerful technique to investigate a manifold of physical and chemical phenomena at the atomic scale. For spin-dependent tunneling, superconducting STM tips are of particular interest due to the well-known spin-polarization of almost 100%, especially in combination with high energy resolution at ultralow temperatures.

We present STM experiments on a V(100) sample in combination with several V-tips at milli-Kelvin temperatures. The applied magnetic fields exceed the critical magnetic field of bulk V, so that the sample is in the normal conducting state. Due to its reduced dimensions the tip apex remains superconducting in fields up to 10 H_c (bulk). Our evaluation of the experimental data is based on Maki's model taking into account effects of orbital depairing and spin orbit coupling [1, 2]. Zeeman splitting of the superconducting quasi-particle densities of states is observed on several V-tips. Further, the quenching process of the superconducting gaps of the V-tips is investigated as function of magnetic fields.

[1] K. Maki, Prog. Theor. Phys. 32, 29 (1964)

[2] R. Meservey et al., Phys. Rev. B 11 4224 (1975)

O 31.5 Tue 11:30 H33

Wave function imaging of transition metal impurities near the H/Si(111) surface — •Benjamin Geisler and Peter Kratzer — Fakultät für Physik and Center for Nanointegration, Universität Duisburg-Essen, 47048 Duisburg, Germany

Despite the difficulties encountered in fabricating magnetic semiconductors, doping of silicon by 3d transition metals is an interesting topic in the field of spintronics. Imaging of electronic states on the atomic scale is possible with state-of-the-art scanning tunneling microscopy (e.g., Jancu *et al.*, PRL 2008, for Mn:GaAs) and can improve the understanding of impurity-host and impurity-impurity interactions.

Here we present an *ab initio* viewpoint on Cr, Mn and Fe impurities near the H/Si(111) surface, which has the specialty of providing a similar chemical environment as bulk Si does, while keeping the impurities accessible to surface analysis techniques. According to our calculations, subsurface doping through the H layer is possible. We discuss magnetic and energetic characteristics of isolated impurities and their detection with (magnetic) scanning tunneling microscopy, which is able to discriminate between interstitial and substitutional defects of different depth. Furthermore, delta layers and 2D clusters of interstitial impurities and their magnetic properties are shown. We find that the impurity wave functions are less extended than those of Mn in GaAs, which makes it harder to get ferromagnetic coupling in Si.

O 31.6 Tue 11:45 H33

First-principles investigation of self energies and theoretical magnetic excitation spectra — •Benedikt Schweflinghaus[1], Manuel dos Santos Dias[1], Antonio Costa[2], and Samir Lounis[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Instituto de Física, Universidade Federal Fluminense, 24210-340 Niteroi, Rio de Janeiro, Brazil

Access to magnetic excitation spectra of single atoms deposited on surfaces is nowadays possible by means of low-temperature inelastic scanning tunneling spectroscopy, see e.g. [1]. A theoretical description of these spectra is accessible through the self energy which describes the coupling of the tunnelling electrons and the spin excitation within the adsorbate. We compute this quantity from first-principles utilizing the Korringa-Kohn-Rostoker Green function method combined with time-dependent density functional theory.

We will present results obtained for single 3d transition-metal adatoms placed on Cu(111) as well as on Pt(111) and proceed to a comparison with available experimental data. In particular, we will show how the imaginary part of the self energy, which essentially describes the lifetime of the excitation, is related to the local density of states as well as to the local dynamical magnetic susceptibility.

This work is supported by the HGF-YIG Programme (VH-NG-717 Funsilab).

[1] A. A. Khajetoorians et al., Phys. Rev. Lett. 106, 037205 (2011)

O 31.7 Tue 12:00 H33

Anisotropic charge oscillations induced by non-magnetic impurities on Fe/W(001) — •Mohammed Bouhassoune, Bernd Zimmermann, Phivos Mavropoulos, Daniel Wortmann, Peter H. Dederichs, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

It has been shown recently that impurities embedded in the surface of few monolayers of Fe deposited on W(001) can trigger intriguing anisotropic charge oscillations [1]. This behavior exhibits a strong dependence on the thickness of the Fe film. Combining first-principles methods: the full-potential linearized augmented plane waves method [2] and the full-potential Korringa-Kohn-Rostoker Green function method [2], we investigate this peculiar behavior by considering single oxygen impurities and find that the anisotropic focused charge oscillations are substantially spin-dependent and are only present when the thickness of the Fe film equals 3 monolayers. We relate this effect to spin-dependent features of the two-dimensional Fermi contours that are crucially affected by the thickness of Fe films.

This work is supported by the HGF-YIG Programme FunSiLab –Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] K. Von Bergmann, PhD Thesis, University of Hamburg (2004)

[2] www.juDFT.de

O 31.8 Tue 12:15 H33

Tunable Kondo resonance of Co atoms on Ag(111) — •maría moro[1,2], david serrate[1,2], marten piantek[3], josé ignacio pascual[4], and manuel ricardo ibarra[1,2] — [1]Instituto de Nanociencia de Aragón and Laboratory for Advanced Microscopy, University of Zaragoza, Spain — [2]Dpto. Física de Materia Condensada, University of Zaragoza, Spain — [3]Instituto de Ciencias de Materiales de Aragón (ICMA), Spain — [4]Nanoscience Cooperative Research Center (CIC Nanogune)

The magnetic properties of atoms on metals are inherently connected with manybody interactions between the localized magnetic moment and the supporting surface. The Kondo effect is the one most frequently found. The energy scale of a Kondo ground state depends strongly on the exchange coupling between atom and surface and, consequently, on the surface local density of states at the Fermi level (LDOS). Here, we study the effect of the LDOS on the magnetic ground state of Co atoms on Ag(111) by constructing artificial atomic structures, which confine surface states electrons and modulate in a predesigned manner the LDOS. By intentionally placing individual atoms at sites with difference LDOS, the Kondo temperature can be varied between 60 to 145 K, demonstrating the precise control of the substrate LDOS is crucial for quantitative analysis of the Kondo state.

O 31.9 Tue 12:30 H33

Controlling spin stability by a vector magnetic field and atom manipulation — •Deung-Jang Choi[1,2], Shichao Yan[1,2], and Sebastian Loth[1,2] — [1]Max Planck Research Group-Dynamics of Nanoelectronic Systems, Center for Free-Electron Laser Science, Hamburg — [2]Max Planck Institute for Solid State Research, Stuttgart

A time-resolving sub-Kelvin scanning tunneling microscope (STM) is used to manipulate atoms and build nanostructures such as atomic chains or arrays. We show that not only static but also dynamic properties of nanostructures can be controlled. We place magnetic atoms into close proximity of existing nanostructures. This modifies available spin relaxation pathways. The resulting variations in the spin relaxation times and spin polarization can be monitored by an all-electronic pump-probe technique [1]. In this way even weak spin coupling can be detected. A vector magnetic field provides additional control over the mixing of spin states without changing the atomic configuration of a nanostructure. For example, we compare the angular dependence of the spin anisotropy for individual Fe atoms and Fe in few-atom arrays. The combination of vector magnetic fields with atom manipulation provides a great deal of control over the behavior of atomic spins making it possible to study spin dynamics at atomic dimensions.

[1] S. Loth, M. Etzkorn, C. P. Lutz, D. M. Eigler, A. J. Heinrich, Science 329, 1628 (2010).

O 31.10 Tue 12:45 H33

Atomically assembled antiferromagnets — •Sebastian Loth — Max Planck Research Group-Dynamics of Nanoelectronic Systems, Center for Free-Electron Laser Science, Hamburg — Max Planck Institute for Solid State Research, Stuttgart

When atoms are placed into regular arrays their magnetic moments can interact and form long-range ordered magnetic states. In particular antiferromagnetic spin coupling creates a large variety of possible collective states. We use low-temperature scanning tunneling microscopy to construct few-atom antiferromagnets. Their shapes can be defined precisely by atom manipulation. In this way uncompensated magnetic moments at the nanoparticle's edge can be avoided. We use such spin-compensated atomic arrays to study the intrinsic dynamics of nanoscale antiferromagnets [1]. For two-dimensional arrays of growing size we can trace the transition from the quantum mechanical singlet ground state to doubly degenerate Neel-type states. Arrays with ten or more atoms can be stable in each state for several hours but current-induced switching between the metastable spin states proceeds at nanosecond speed. These properties enable a model demonstration of dense magnetic data storage using antiferromagnets memory elements.

[1] S. Loth, S. Baumann, C. P. Lutz, D. M. Eigler, A. J. Heinrich, Science 335, 196 (2012).

O 31.11 Tue 13:00 H33

Epitactical grown Kondo lattices spanning different localization regimes of the Ce 4f electrons — •Holger Schwab, Mattia Mulazzi, and Friedrich Reinert — Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg, Germany

Ce surface alloys promise to be the choice of materials to study transformations of the electronic band structure during low temperature phase transitions in Kondo lattices. [1] The low temperature behaviour of Ce based Kondo systems strongly depends on the energy scales in the Ce atom and the hybridization between the Ce 4f orbitals and the conduction band. [2] Probing the Ce 4f spectral function [3] or the Ce 3d states therefore allows to preliminarily characterize and select such compounds. With XPS (X-ray Photoelectron Spectroscopy) of the Ce 3d states we investigated Ce surface alloys on Ag(111), Pt(111) and Pd(111) surfaces. Based on a GS-fit [4] to these data we were able to compare and rank the parameters responsible for the behaviour of these alloys in the single impurity regime of the Kondo lattice.

[1] M. Klein et al.,Phys. Rev. Lett. 106, 186407 (2011), P. Coleman, Science 327, 969 (2010)
[2] F. Patthey et al., Phys. Rev. B 42, 8864 (1990)
[3] H. Schwab et al., Phys. Rev. B 85, 125130 (2012)
[4] O. Gunnarsson et al., Phys. Rev. B 28, 4315 (1983)

O 32: Metal Substrates I

Time: Tuesday 10:30–12:30 Location: H42

O 32.1 Tue 10:30 H42

Energy transfer in inert gases-substrate interactions studied by Pt-SiOx-Si chemoelectronic thin film devices — •Michael Scheele, Ievgen Nedrygailov, Eckart Hasselbrink, and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, 45117 Essen, Germany

Energy flow in chemical surface reactions comprise excitation and relaxation of reacting molecules as well as heating and electronic excitation of the substrate. On the other hand, molecules can also take up energy from a heated substrate. Both, energy loss of molecules to the substrate as well as energy take up from the substrate can be detected by means of chemoelectronic devices. These devices are thin film metal-semiconductor or metal-insulator-metal junctions with a top metal electrode of nanometer thickness acting as the substrate. The energy transfer from a heated metal film to a molecular beam of argon, helium or nitrogen can be monitored as a change of the device current driven by a constant bias voltage. The current changes can be a result of a temperature difference across the device. The sensitivity of the device can be tuned by the magnitude and the polarity of the bias voltage and the base temperature of the device.

O 32.2 Tue 10:45 H42

SPALEED and STM studies of the reconstructed Au(100) surface — •Rene Hammer[1], Anke Höfer[1], Mario Kiel[1], Klaus Meinel[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck Institut für Mikrostrukturphysik, D-06120 Halle, Germany

The hexagonal reconstruction of Au(100) has been intensively studied over more than four decades [1]. Nevertheless, some issues regarding the toplayer to substrate matching and alignment, respectively, are ambiguously reported. We quantitatively reinvestigated the system by combining the high resolving powers of SPALEED and STM. A Au(100) sample of excellent quality was used showing after cleaning two types of perfect c(26x48) superstructure domains. They are generated by the buckling of quasihexagonal toplayers which are characterized by lattice vectors having the length of 0.9575a and 0.9630a, respectively, where a is the interatomic distance of Au(100). The former vectors exactly run along [011] or [01-1] whereas the latter ones deviate by 120.19° from that directions. Ar^+ ion bombardment at elevated temperatures induced a rotation of the toplayers up to angles of ± 0.89°. Sample annealing yields a turning back into the initial toplayer alignment. The reorientation proceeds continuously, i.e. all angles between ± 0.89° are observed.

[1] D.G. Fedak and N.A. Gjostein, Surf. Sci. 8 (1967) 77; M.A. Van Hove et al., Surf. Sci. 103 (1983) 189; G.K. Binnig et al., Surf. Sci. 144 (1984) 321; P. Havu et al., Phys. Rev. B 82 (2010) 161418(R).

O 32.3 Tue 11:00 H42

Electron pair emission from Ag(100) — •Lucie Behnke[1], Frank O. Schumann[1], and Jürgen Kirschner[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle/Saale — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle/Saale

A recent (e,2e) study on a Cu(100) surface revealed the importance of pair diffraction. A kinematic pair diffraction model described the results reasonably well. The approach is justified by current (e,2e) theory, which characterizes the in-coming and out-going electrons by LEED and time reversed LEED-states, respectively. To explore the validity of the kinematic model, the experiment was repeated with a Ag(100) crystal. We have systematically studied the electron pair emission from the surface as a function of the primary energy (E_p = 30 eV to 67 eV). An improvement to the previous experiment is the ability to measure the primary electron flux. This allows to determine the single/coincidence count rate per incoming electron. In addition, we identify contributions from valence states of different orbital characters. The spectra can be divided into three regions with the help of a theoretical band structure calculation. We focus now on the region near E_f, which has a low DOS. However, in the experiment high intensities were measured. Moreover, the relative spectral contribution from the electrons near E_f is strongly affected by the primary electron energy and display a non-monotonic behavior. The origin of these variations and the similarities and differences with respect to the Cu(100) surface will be discussed.

O 32.4 Tue 11:15 H42

Electromechanical coupling coefficients of sp-bonded metals from first principles — •Anja Michl[1,2], Jörg Weissmüller[1,3], and Stefan Müller[2] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — [3]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Coupling between mechanical stress or strain of a surface and its electronic properties is relevant for a range of applications from sensors and actuators to heterogeneous catalysis. In experiment, coupling coefficients are determined via electrochemical experiments, e.g. by measuring the change in electrode potential upon applying tangential strain e to the electrode surface. Theoretically, this coupling strength is obtained as the response of the electronic work function W to strain. Thus, we calculate strain response parameters $\mathrm{d}W/\mathrm{d}e$ for several sp-bonded metals from first principles using density functional theory. We find an increasing trend for the coupling coefficients with increasing number of valence electrons. For aluminum the sign is inverted leading to abnormal positive response parameters for all orientations considered. Due to the simple sp-bonded electronic structure of the investigated metals the homogeneous electron gas represents a suitable model system. Based on an analysis of the surface and volume contributions of the work function within the framework of this jellium model, we propose the unusual positive sign to be related to the high electron density of aluminum.

O 32.5 Tue 11:30 H42

Ab-initio modeling of electromechanical coupling at Si surfaces — •Sandra Hoppe[1], Anja Michl[1,2], Jörg Weissmüller[2,3], and Stefan Müller[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [3]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Electrochemical experiments have revealed a linear dependence of the electrode potential E of metal surfaces on an applied strain e. This electromechanical coupling is characterized by the response parameter $\partial E/\partial e = const =: \varsigma$. As the potential of zero charge of an electrode surface in electrolyte is closely linked to its work function W in vacuum, ς is accessible via ab-initio calculations of $\partial W/\partial e$. The response of the work function to strain has been investigated experimentally and in theory for various metals. In order to gain further insight into the influence of the electronic structure on the work function strain response, we have calculated coupling coefficients for silicon surfaces. Density functional theory with the HSE screened hybrid exchange-correlation functional was applied to obtain accurate Si band structures. In contrast to most metal surfaces, the magnitude of the response parameters does not increase with packing density for Si. This phenomenon is discussed regarding the strongly directional covalent semiconductor bonds and their distortion under applied strain.

O 32.6 Tue 11:45 H42

Fe3Al surfaces in dry and humid oxygen atmosphere — •afshin izanlou, mira todorova, martin Friák, and jörg neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The elastic and corrosion properties of iron-aluminides make them interesting candidates for high temperature applications, but the degradation of these properties at room temperature and in the presence of hydrogen hinder their utilisation. Aiming to understand the mechanisms and interactions, which have such negative impact on the properties of these materials, we study the low-index surfaces of Fe3Al in dry and humid oxygen environment, combining density-functional theory with thermodynamic considerations. We find mixed terminated surfaces, i.e. containing both Fe and Al, to be most stable and a marked preference for oxygen adsorption in an aluminium rich environment. This result correlates nicely with the observation that Al2O3 is the thermodynamically stable oxide, when these surfaces come into contact with oxygen. Water, on the other hand, favours adsorption on Fe, on which it adsorbs with the oxygen end. Consequences for the corrosion behaviour and protection of these surfaces will be discussed.

O 32.7 Tue 12:00 H42

Interactions of oxidizing species with the Mg(0001) surface: the role of electrostatic contributions — •Su-Ting Cheng, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH

The adsorption of oxidizing species {N,O,F, Cl} on the Mg (0001) surface were studied using density functional theory. We observe a negative adsorbate-induced work function change and an increase in the binding energy with increasing adsorbate coverage, both of which fail to comply with common expectations regarding the adsorption of electronegative elements on a metal surface. Analysing the electronic structure we are able to explaine these changes in terms of a redistribution of electrons at the surface, which lowers the surface dipole. We find a correlation between the efficient embedding of the electronegative adsorbates into the electron spill-out from the Mg surface and the size of the adsorbate atoms. The special reduction of the electron spill-out furthermore causes a decrease in the electrostatic energy which dominates the binding energy within the studied adsorption system. The impact of these unusual trends on metal corrosion will be discussed.

O 32.8 Tue 12:15 H42

Joint DFT and STM/LEED investigation of oxygen adsorption on Ir(100)-1x1 — •Anja Michl[1,2], Pascal Ferstl[3], Tobias Schmitt[3], Lutz Hammer[3], M. Alexander Schneider[3], and Stefan Müller[2] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — [3]LS f. Festkörperphysik, Universität Erlangen-Nürnberg, Germany

We explore the structure and stability of oxygen overlayers on Ir(100)-1x1 by combining first-principles calculations using density functional theory (DFT) with LEED and STM. The energetics of various ordered superstructures with different adsorption sites and coverages θ are used to construct a surface phase stability diagram. Apart from the well-known (2×1)-br superstructure and a (hypothetical)(1×1)-br phase, we identify two more ground states, which are also characterized by oxygen atoms exclusively occupying bridge positions: a (3×1)-br structure at $\theta = 0.33$ ML and a (4×1)-3br with 3 O-atoms per unit cell at $\theta = 0.75$ ML. Both new phases are verified by experiment, whereby the (3×1)-br structure could be prepared as single phase all over the surface, while the (4×1)-3br was found only as small patches of locally higher coverage within the (2×1)-br phase. Moreover, periodically arranged 1D domain walls with locally reduced oxygen coverage are observed with STM. We compare different models for the atomic structure of the domain walls based on a shifted row reconstruction mechanism of the underlying iridium substrate.

O 33: Nanostructures at Surfaces III

Time: Tuesday 10:30–12:45 Location: H45

O 33.1 Tue 10:30 H45

Surface modification on ultra-thin sheets of molybdenum disulfide due to irradiation with highly charged ions — Johannes Hopster, •Roland Kozubek, Jakob Krämer, and Marika Schleberger — Universität Duisburg-Essen, Duisburg, Deutschland

This presentation deals with the interaction of highly charged ions with single layer molybdenum disulfide. For this purpose MoS_2 was exfoliated on a (100)-Potassium bromide crystal and afterwards irradiated with xenon ions. Xe^{35+} and Xe^{40+} were used while the kinetic part of the energy was kept constant. By means of atomic force microscopy, pits and hillocks could be identified. The creation of hillocks was observed for both charge states and for different thicknesses of the MoS_2 layers, while their height and diameter depend on these aforementioned values. The different illustration of the defects obtained in trace and retrace scan direction in contact mode lead us to believe, that at this positions an enhanced friction exists, while the information of the topography arises from the tapping mode measurements.

The creation of pits could only be observed on single layer MoS_2 after the irradiation with Xe^{40+}. Because of the fact that the ion induced defects on KBr are quiet similar to the detected ones we deduce that these pits are formed underneath the single layer in the substrate. As a consequence, the MoS_2-Layer at this position could also be damaged and demolished.

O 33.2 Tue 10:45 H45

Novel approach to the fabrication of mixed monomolecular films and chemical patterns — •M Nuruzzaman Khan and Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

Self-assembled monolayes (SAMs) provide a convenient and flexible means to control surface properties by covering surfaces with chemically uniform and densely packed monomolecular films. A versatile approach to prepare mixed SAMs and SAM-based chemical patterns on coinage metal substrates is irradiation promoted exchange reaction (IPER). The key idea of this approach is tuning the extent of the exchange reaction between a SAM covering the substrate and a potential molecular substituent by electron irradiation. As such substituents, different thiols are usually used. Here we show that not only thiols but also disulfides can serve as substituents in IPER, which extends significantly the possibilities of this approach, making it suitable for another class of commercially available compounds. Using several model disulfide compounds, we studied the outcome and kinetics of IPER in this particular case and compared them with the analogous performance of thiols. Additionally, the approach was combined with electron beam lithography and applied to the fabrication of chemical patterns which were amplified in the z-direction by surface initiated atom transfer radical polymerization.

O 33.3 Tue 11:00 H45

On the interaction of ultrathin porphyrin layers with high energy electrons — •Florian Vollnhals, Patrick Wintrich, Marie-Madeleine Walz, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander-University Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

The interaction of energetic electrons with matter is of general interest for many fields in science and technology. In this contribution we investigate the effect of electron irradiation on monolayer and multilayer films of porphyrin derivatives adsorbed on a Ag(111) single crystal using Scanning Tunneling Microscopy (STM) and Scanning Electron Microscopy (SEM) in ultra-high vacuum (UHV). We find that the corresponding electron induced defects first of all depend on the thickness of the organic film and secondly can be used for further development to fabricate metallic nanostructures. The observed effect is closely related to the novel Electron Beam Induced Surface Activation (EBISA) technique recently explored by our group. In EBISA, an oxide surface, e.g. SiO_2, is irradiated by a focused electron beam, resulting in the chemical activation of the area, such that successively dosed $Fe(CO)_5$ is decomposed and forms an iron deposit. Further autocatalytic growth results in pure (>90%at.) crystalline iron nanostructures.[1] In this contribution we expand this concept to porphyrin layers on Ag(111) as a novel means to fabricate complex nanostructures with lithographic control. This work was supported by the DFG via grant MA 4246/1-1.

[1] M.-M. Walz et al., Angew. Chem. Int. Ed. 49 (2010), 4669

O 33.4 Tue 11:15 H45

Interlayer formation of Diamond-Like Carbon Coatings on Polyethylene Plastic Material — •Christian B. Fischer[1], Magdalena Rohrbeck[1], Stefan Wehner[1], Matthias Richter[2], Matthias Städter[2], and Dieter Schmeisser[2] — [1]Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany — [2]Department of Applied Physics and Sensors, Brandenburg University of Technology, 03046 Cottbus, Germany

The coating of materials with diamond-like carbon (DLC) is a very common way to further improve and modify surface specific properties. Although DLC is frequently used as a protective coating on several substrates, the chemical and physical properties throughout the coating process on plastics are yet sparsely investigated. Different layer thicknesses of two types of protective coatings one sp3-enriched (robust, r-type) and one with more sp2-centers (flexible, f-type) have been realized on polyethylene by PECVD. Microscopic analysis showed diverse surface topographies for the two DLC-types. NEXAFS spectroscopy revealed significant details of carbon centers in chemically different neighborhood displaying a characteristic fingerprint behavior. The appropriate explanation for the current carbon deposition process is obviously the formation of an interlayer between these unequal materials. An improved understanding of hard DLC and soft polyethylene assembly is part of the present work.

O 33.5 Tue 11:30 H45

A new route for the electroless fabrication of mesoporous silicon — •Xiaopeng Li[1,2], Stefan L. Schweizer[2], Alexander Sprafke[2], and Ralf B. Wehrspohn[2,3] — [1]Max-Planck Institute of Microstructure Physics, Halle D-06120, Germany — [2]Martin-Luther-University Halle-Wittenberg, Germany — [3]Fraunhofer Institute for Mechanics of Materials, Halle D-06120, Germany

Recently, mesoporous silicon (meso-PSi) has demonstrated considerable potential for bio-medical applications regarding biocompatibility and biodegradability, due to its large internal surface area and its mechanical stability. In photovoltaics, meso-PSi has been utilized for antireflective layers, and as sacrificial layers for layer-transfer processes. Until now, electrochemical etching (ECE) is considered as the only method to achieve controlled fabrication of meso-PSi. However, ECE is cost-inefficient on full wafer-scale, additionally, its process stability for high-throughput, in-line processes is critical on wafer-scale. Here, we present a new route for the fabrication of meso-PSi using Pt nanoparticle-assisted chemical etching (PaCE) without applying any external potential. Si wafers were firstly loaded with Pt nanoparitcles (PtNPs), and then immersed in solution containing HF and H2O2. PtNPs drill nanopores deep into the Si substrate; meanwhile, meso-PSi is created. The obtained mesoporous silicon films show surprisingly good uniformity in which the porosity and thickness can be tuned well via adjusting the etching conditions. To qualitatively explain the observed phenomenon, we propose a new model based on the Pt-Si nano-Schottky contact.

O 33.6 Tue 11:45 H45

Emission cone narrowing of electrons in the strong field around a sharp metallic nanotip — Doojae Park, Björn Piglosiewicz, Slawa Schmidt, •Petra Gross, and Christoph Lienau — Ultraschnelle Nano-Optik, Institut für Physik, Universität Oldenburg, 26111 Oldenburg

When sharp, nanometer-sized metal tips are irradiated with few-cycle near-infrared laser pulses with around 1.6 μm center wavelength and few nJ energy, the strong laser field around the tip apex enables tunneling of electrons out of the tip. At these conditions, we find a pronounced strong-field acceleration of the electrons within the field gradient near the tip apex, and we observe a distinct narrowing of the emission cone angle of the fastest electrons.

We investigate the electron motion in the strong field around the nanostructure by recording angle-resolved kinetic energy spectra and using numerical simulations incorporating the curved, vectorial gradient of the oscillating laser field [1]. These studies show that the emission cone narrowing of the fastest electrons can be ascribed to the field-induced steering of sub-cycle electrons, which escape the tip's near field within half an oscillation of the laser pulse. Our results indicate new possibilities for designing directional ultrafast electron sources.

[1] D. J. Park *et al.*, Phys. Rev. Lett., in press (2012)

O 33.7 Tue 12:00 H45

Electron motion in few-cycle laser field around metallic nanostructures — Björn Piglosiewicz, Slawa Schmidt, Doojae Park, Jan Vogelsang, •Petra Gross, and Christoph Lienau — Ultraschnelle Nano-Optik, Institut für Physik, Universität Oldenburg, 26111 Oldenburg

Sharp metallic nanotips irradiated with few-cycle laser pulses are promising candidates as sources of highly confined electron wavepackets of short temporal duration and high spatial directivity. Specifically the strong-field regime, where electron emission by tunneling becomes dominant over multi-photon and above-threshold ionization, enables the generation of (sub-)femtosecond electron wavepackets. For sufficiently long wavelengths and short pulses, electrons are accelerated to escape the near field within one half-cycle of the laser oscillation [1,2].

Here, we study for the first time the effect of the carrier envelope phase of few cycle laser pulses on the motion of electrons emitted from metallic nanostructures by strong-field tunneling. Sharp gold tips are illuminated with CEP-stable few-cycle near-IR pulses at 1.5 μm and the kinetic energy spectra of the emitted electrons are recorded. We observe pronounced modifications of the photoelectron spectra when varying the CEP phase. Our results, explained within a modified Simpleman model, shed new light on the light-driven motion of electrons in the near field of metallic nanostruuctures on sub-femtosecond time scales.

[1] G. Herink *et al.*, Nature **483**, 190 [2012]

[2] D. J. Park *et al.*, Phys. Rev. Lett., in press (2012)

O 33.8 Tue 12:15 H45

DNA-Modulated Heterogeneous Nucleation and Growth of Functional Silver Nanoparticles on AgCl Particle Surface — •Guoqing Wang[1], Hideyuki Mitomo[2], Yasutaka Matsuo[2,3], Kenichi Niikura[2,3], and Kuniharu Ijiro[2,3] — [1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, N13W8, Sapporo 060-8628, Japan — [2]Research Institute for Electronic Science, Hokkaido University, N21W10, Sapporo 001-0021, Japan — [3]JST-CREST, Sanban-cho 5, Chiyoda-Ku, Tokyo 102-0075, Japan

Photocovnersion of AgX (X = Cl, Br, I) to functional silver nanoparticle (AgNPs) is of both scientific curiosity and technological importance. Here we show that AgCl can be photoconverted to AgNPs within minutes via photoreduction in the presence of DNA. Our mechanistic studies reveal that the heterogeneous nucleation and growth of AgNPs on AgCl correlates well with the thermodynamic explanation in terms of a reduced interfacial energy barrier, and DNA serving as a template plays an essential role in controlling the morphology and size of the AgNPs. The resultant AgNPs are observed to be biofunctionalized, and exhibit photostable luminescence and DNA-specific surface-enhance Raman scattering (SERS) signature, allowing for DNA-directed recognition and dual-modal cell imaging. Furthermore, DNA-encapsulated Ag/AgCl nanostructures can be obtained through a short-term photoreduction. Their uses in plasmonic photocatalysis are demonstrated.

O 33.9 Tue 12:30 H45

Scanning probe microscopy and spectroscopy of nanodiamonds under illumination. — •Rémy Pawlak[1], Thilo Glatzel[1], Shigeki Kawai[1], Sweetlana Fremy[1], Loïc Schmidlin[2], Vincent Pichot[2], Denis Spietzel[2], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland. — [2]Nanomatériaux pour des Systèmes Sous Sollicitations Extrêmes (NS3E) UMR 3208 ISL/CNRS Institut franco-allemand de recherches de Saint-Louis (ISL), 5 rue du Général Cassagnou, 68300 Saint-Louis, France.

Nanodiamonds (ND) are carbon particles with size from 2 to few tens of nanometers which already have broad applications in polishing materials, lubricants as well as applications in biomedical imaging. More recently, the accurate control of the doping of the nanodiamond structure with atomic defects,such as Nitrogen-Vacancy centers (NV-1), having optical and spin properties gives to this material an exceptional candidate for photonic devices and quantum information processing and computing. Here, we combine scanning probe microscopy imaging and spectroscopy to investigate at the atomic scale single nanodiamonds/HOPG. Under illumination with wavelenghts of 400 nm and 470 nm, a modulation of the electronic band gap as well as the contact potential difference (CPD) between tip and sample is observed compared to the dark condition, whereas no relevant variation is obtained for wavelenghts superior to 590 nm. This effect is a direct evidence of the light-induced charges arising from the NV centers of nanodiamonds.

O 34: Invited Talk (Martin Weinelt)

Time: Tuesday 15:00–15:45 Location: H36

Invited Talk O 34.1 Tue 15:00 H36

Ultrafast Spin and Magnetization Dynamics and their Signatures in the Transient Band Structure — •Martin Weinelt — Freie Universität Berlin, Germany

Femtomagnetism is now an established and active research field in thin film and surface magnetism, which promises magnetic writing speeds three orders faster than current technology. Investigations in this area comprise the spin and magnetization dynamics in ferro- and ferrimagnetic samples initiated with a femtosecond laser pulse. In the first two picoseconds after optical excitation the electronic system and the underlying lattice and spin subsystems are not in equilibrium and it seems likely that the transient hot electron population is responsible for the ultrafast change of the magnetization. Still it remains controversial, which microscopic processes are fast enough to provoke femtomagnetism: direct interaction with the laser field, scattering among electrons, phonons and magnons, and/or spin-transport? We approach these problems with time- and angle-resolved photoemission (TR-ARPES) using lasers and high-order harmonics XUV sources. The spin dependence of electron scattering processes is investigated for the 3d band ferromagnets. Ultrafast demagnetization is studied for the local-moment ferromagnets Gadolinium and Terbium. Here equilibration of the excited state involves more than one timescale, because the optical excitation occurs in the valence band but the magnetic moment is dominated by the localized 4f electrons. Following excitation by an intense infrared pulse, TR-ARPES allows us to map the transient exchange splitting of the valence bands in the 3rd Brillouin zone.

O 35: Poster Session I (Metal, semiconductor and oxide substrates: structure and adsorbates; Graphene)

Time: Tuesday 18:15–21:45 Location: Poster B1

O 35.1 Tue 18:15 Poster B1

Electronic structure of Ag(100) revisited by STS — •Robin Ohmann[1], Cormac Toher[1], Jörg Meyer[1], Anja Nickel[1], Francesca Moresco[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — [2]Division of IT Convergence Engineering, POSTECH, Pohang 790-784, Republic Korea

The Ag(100) surface is used for many surface science studies as a substrate. Therefore, a clear knowledge about its electronic properties is desirable. In contrast to previous results, we present an experimental study on Ag(100) revealing an electronic state, at which electrons behave like in a two-dimensional electron gas. Conductance maps taken with scanning tunneling spectroscopy (STS) show energy dependent standing wave patterns at step edges and defects, from which the dispersion relation is extracted. We find a parabolic behaviour with a state onset of 1.9 eV above the Fermi energy and an effective mass of 0.41 m_e. Scanning tunneling spectra reveal a clear feature at the relevant energy. Additionally, the lifetime, linewidth and coherence length have been measured as a function of energy. Theoretical calculations have been performed to elucidate the experimental findings.

O 35.2 Tue 18:15 Poster B1

Electron pair emission from surfaces upon He^{2+} impact — •Chang-Hui Li[1], Christian Tusche[1], Frank O. Schumann[1], and Jürgen Kirschner[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

Using a two-electron coincidence spectrometer, we have studied the electron pair emission upon the impact of 10 eV normal incident He^{2+} ions on Ir(100) and Fe(100)-p(1×1)O surfaces. According to the commonly used two-step model [1], He^{2+} is firstly converted to He^{+} and then to He^{0}. Two electrons are emitted incoherently by the two corresponding neutralization steps. As the ionization potentials of He^{2+} → He^{+} and He^{+} → He^{0} are 54.4 eV and 24.6 eV, respectively, a very unequal energy sharing is expected. In the two-electron coincidence spectra, the dominant events can be understood by the incoherent two-step mode, but we have found clear evidence that this approximation breaks down and the neutralization should be treated as a single process.

[1] P. A. Zeijlmans van Emmichoven, P. A. A. F. Wouters, and A. Niehaus, 1988 Surf. Sci. 195 115

O 35.3 Tue 18:15 Poster B1

A LEED investigation of the Au(111)-(1×1) surface — Birgit Vogt and •Jochen Vogt — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Although the ground state of the clean Au(111) surface shows reconstruction [1], the latter can be lifted, e. g. electrochemically, by stress, or by the presence of surface imperfections. For the clean unreconstructred Au(111)-(1×1) surface, both a layer distance compression as well as an anomalous layer distance expansion have been proposed at the solid vacuum interface [2,3]. We have prepared and characterized clean Au(111) surfaces by means of LEED, STM, XPS, and AES. The softly-annealed surfaces exhibit bright LEED diffraction patterns of (1×1) symmetry over a large energy range up to 450 eV. The measured diffraction beam intensities as a function of electron energy were the basis of a surface structure analysis. The structural results for the Au(111)-(1×1) surface are discussed in the context of reported structure data in literature and possible sources of error.

[1] S. B. Darling et al., Langmuir 18 (2002), 7462
[2] G. M. McGuirk et al., 10th International Conference on the Structure of Surfaces, 2011
[3] L. Guan et al., Solid State Commun. 149 (2009), 1561

O 35.4 Tue 18:15 Poster B1

One-step or two-step core-resonant double photoemission from a Ag(100) surface — •Zheng Wei[1], Frank O. Schumann[1], Changhui Li[1], Lucie Behnke[1], Gianluca Di Fillippo[2], Giovanni Stefani[2], and Jürgen Kirschner[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany — [2]CNISM andDipartimento di Fisica, Università Roma Tre, I-00146 Rome, Italy — [3]Martin-Luther Universität, 06120 Halle, Germany — [3]Martin-Luther Universität, Halle,Germany

We studied core-resonant double photoemission (DPE) from a Ag(100) surface with coincidence electron spectroscopy, and mapped out the two-dimensional energy distribution of the DPE pairs. Our experiments demonstrate that the photo-excited Auger transitions involving the Ag $M_{4,5}$ core levels can be described by a simplified two-step picture, while the Auger transitions involving the Ag $N_{2,3}$ core levels can only be described by a one-step picture. Since the final states of both Auger transitions are the same, this variation is purely due to the different initial core-hole state with different lifetime. We experimentally extracted the intrinsic line shapes of the $M_{4,5}VV$ Auger spectra, and found out the spectral weight transfer of the $^3F_4$ component from the atomic- to the band-like region.

O 35.5 Tue 18:15 Poster B1

Pattern formation of Ni- and Fe-Tetramethyl-tetraazaanulene on Au(111) — •Thomas Knaak[1], Thiruvancheril G. Gopakumar[1], Bettina Schwager[2], Felix Tuczek[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [2]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel

Saddle shaped Ni- and Fe-tetramethyl-tetraazaannulene (TMTAA) on Au(111) were investigated using low-temperature STM. Surprisingly, we observed the formation of different patterns, depending on the central ion, Ni or Fe. While Ni-TMTAA aggregates at low coverages into chiral clusters, Fe-TMTAA molecules remain isolated from each other and arrange in a hexagonal array. Presumably, different degrees of bending of TMTAA due to Ni and Fe is the origin of the different aggregation behaviors. Financial support by the Deutsche Forschungsgemeinschaft via the SFB 677 is acknowledged.

O 35.6 Tue 18:15 Poster B1

Intramolecular resolved STM-data of Biphenyldithiol-molecules on Au(111) — •Michael Lochner, Michael Waelsch und Rene Matzdorf — Universität Kassel, Fachbereich Naturwissenschaften,

We have investegated submonolayers of the organic molecule Biphenyldithiol on an Au(111)-surface with STM-methods. The molecules are physisorbed on the surface. Three types of typical structures have been found, which are dependent on the local coverage. We show intramolecular resolved data of molecules in all three structures. Additionally, workfunction-maps were measured by lock-in-technique. In some cases they show even more details of the molecule structure than usual STM-topographies.

O 35.7 Tue 18:15 Poster B1

Final-State Diffraction Effects In Angle-Resolved Photoemission At An Organic-Metal Interface — •Bocquet F. C.[1,2], Giovanelli L.[2], Amsalem P.[3], Petaccia L.[4], Topwal D.[4], Gorovikov S.[4], Abel M[2], Koch N.[3], Porte L.[2], Goldoni A[4], and Themlin J.-M.[2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Aix-Marseille Univ, IM2NP, 13397 Marseille, France — [3]Institut fur Physik, Humboldt-Universitat zu Berlin, 12489 Berlin, Germany — [4]Sincrotrone Trieste, 34149 Trieste, Italy

The growth of organic thin films on metallic substrates has become a field of growing interest for organic electronics as well as for fundamental surface science [1]. We show that angle-resolved photoemission performed using low-energy photons on an organic-metal interface allows to clearly distinguish genuine interface states from features of substrate photoelectrons diffracted by the molecular lattice [2]. As a model system, an ordered monolayer of Zn-phthalocyanine is used as a diffraction lattice to probe the electronic band structure of a Ag(110) substrate. Photoemission close to normal emission geometry reveals strongly dispersive features absent in the pristine substrate spectra. Density functional theory modelling helped identifying these as bulk sp direct transitions undergoing surface-umklapp processes. The present results establish the important role of final-state diffraction effects in photoemission experiments at organic-inorganic interfaces.

[1] Bartels, Nature Chemistry 2 87 (2010) [2] Bocquet et al. Phys. Rev. B 84 241407(R) (2011)

O 35.8 Tue 18:15 Poster B1

Kinetic parameters of molecule dynamics and reactions determined with a scanning tunneling microscope at room temperature and above — •Michael Stark, Stefanie Ditze, Martin Drost, Florian Buchner, Elisabeth Zillner, Michael Röckert, Hans-Peter Steinrück, and Hubertus Marbach — LS. f. PC II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The knowledge of kinetic parameters is generally important for a detailed understanding of chemical and physical processes, like the self-assembly of molecular building blocks into supramolecular structures. In this study we investigate the kinetics of surface diffusion and the self-metalation reaction of 2H-tetraphenylporphyrin (2HTPP) on Cu(111). The determination of the corresponding parameters and activation energies is thereby based on experimental data acquired with a scanning tunneling microscope (STM) at room temperature and above in ultrahigh vacuum. One the one hand the focus of this study is on the “slow“ unidirectional diffusion of 2HTPP along the close packed atomic rows of Cu(111) and on the rotation of the latter molecules on the same substrate. We also investigated the surface-mediated self-metalation reaction of 2HTPP with Cu atoms from the Cu(111) substrate. By counting individual molecules in the corresponding ST micrographs we are able to determine the rate constants of this reaction at different sample temperatures and thus to determine the activation energy for the metalation reaction based on these values.

This work has been funded by the DFG through SFB 583

O 35.9 Tue 18:15 Poster B1

Structural and electronic characterization of an adsorbed SMM building block: Cu$_3$-triplesalen on Au(111) — •Judith Niedenführ[1], Manuel Steinbrecher[1], Thorsten Glaser[2], and Daniel Wegner[1] — [1]Westfälische Wilhems-Universität, Münster, Germany — [2]Universität Bielefeld, Bielefeld, Germany

Single Molecule Magnets (SMMs) are potential candidates for the application in future technological devices for high-density memory storage and quantum computation. In an attempt to combine a high spin ground state and a large magnetic anisotropy in one molecule, triplesalen complexes are promising building blocks for a new generation of SMMs. For an efficient superexchange interaction, a delocalized aromatic π system in the center of the triplesalen complex is required. However, previous chemical analysis indicates that the central benzene ring inside this complex can change its configuration to cyclohexane, therefore causing a loss of aromaticity. This has a dramatic impact on the magnetic coupling and spin polarization of the triplesalen complex. Employing a combination of Scanning Tunneling Microscopy (STM) and Scanning Tunneling Spectroscopy (STS) we have investigated single Cu$_3$-triplesalen complexes adsorbed on a Au(111) surface. The relatively large molecules were deposited in situ using a pulse injection technique. A thorough structural and spectroscopic analysis allows us to discuss the electronic properties of the Cu$_3$-triplesalen complex, with a special focus on the state of the central carbon ring.

O 35.10 Tue 18:15 Poster B1

Single Component and Compound Monolayers of CuPc and PTCDA on a Ag(110) Surface — •Kathrin Schönauer[1,2], Martin Willenbockel[1,2], Benjamin Stadtmüller[1,2], Christian Kumpf[1,2], Sergey Soubatch[1,2], and Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology, Germany

Organic semiconductors are of great interest for research due to their potential application in organic electronics. Organic layers of one component on top of a metal crystal have been studied for decades. Recently binary and multinary molecular films also have come into focus, e.g., for the application in organic p-n junctions and all-organic solar cells. Traditionally, (111) surfaces of Ag, Au and Cu single crystals were used for experimental studies. Here we report on the structure of ordered monolayers of CuPc and PTCDA on a Ag(110) surface, both single component and compound. Scanning Tunneling Microscopy and Low Energy Electron Diffraction were used.

O 35.11 Tue 18:15 Poster B1

Wave-function tuning in self-assembled monolayers — •Bernhard Kretz, David Alexander Egger, Elisabeth Verwüster, and Egbert Zojer — Institute of Solid State Physics, Graz University of Technology

The distribution of dipolar groups along phenylthiol-based self-assembled monolayers (SAMs) was shown to cause a modification of the electron wave-function and the vacuum level.[1] In particular the molecular orbitals, like the highest occupied molecular orbital (HOMO) and the lowest unoccupied orbital (LUMO), get shifted in energy and localized. In this work, we perform band structure calculations using density functional theory on phenylthiol-based SAMs where dipolar and non-conjugated groups are distributed along the SAMs. The results indicate that the localization can be supported by breaking the conjugation along the backbone. Analysing the influence of the dipolar and non-conjugated groups on the wave-function guides the way towards a toolbox for wave-function engineering.

[1] F. Rissner et al., J. Am. Chem. Soc. 2011, 133, 18634

O 35.12 Tue 18:15 Poster B1

Impact of disorder on the properties of self-assembled monolayers with embedded dipoles — •Iris Hehn[1], Manuel Vieider[1], Otello Maria Roscioni[2], Luca Muccioli[2], Martin Stolterfoht[1], Michael Zharnikov[3], Claudio Zannoni[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, Viale del Risorgimento, 4, 40136 Bologna, Italy — [3]Applied Physical Chemistry, Heidelberg University, Im Neuenheimer Feld 253, 69120, Heidelberg, Germany

In this work mid-chain ester functionalized alkanethiols adsorbed on a gold {111} substrate are studied using molecular dynamics simulations and density functional theory calculations. The lengths of the alkyl segments above and below the carboxylate dipolar groups as well as the molecular coverage are systematically varied to study the impact of those parameters on the order within the layers. The latter is quantified based on various structural parameters, like tilt-, azimuthal- and twist-angles. To assess the impact of disorder on the electronic properties of the monolayers, histograms of tilt angle and dipole orientation distributions have been calculated and the impact of coverage and molecular structure on charge and potential distributions within the SAMs were studied.

O 35.13 Tue 18:15 Poster B1

PTCDA on Cu(100) re-investigated by STM — •Stefan Gärtner, Benjamin Fiedler, Oliver Bauer, and Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany

Whether the adsorption of an organic adsorbate on a metal surface leads to ordered or disordered structures, possibly including molecular dissociation, depends on the interfacial chemistry. While PTCDA forms long-range ordered structures on all Au and Ag surfaces, different structure models [1,2] and even a molecular dissociation were discussed for PTCDA on Cu(100) on the basis of XPS data [1]. To clarify this we have performed so far missing STM investigations. Indeed, for Cu(100), we find that the preparation of long-range ordered structures requires elevated sample temperatures (400 K), pointing to a considerable corrugation of the surface bonding potential. However, from the STM images, we obtain no indications for dissociation. We put forward a structure model with an L-type arrangement of the molecules in the monolayer and the second layer in agreement with the proposed $(5\sqrt{2} \times 4\sqrt{2})R45^\circ$ structure of ref. [1]. The lattice parameters of this model are in full agreement with our LEED results on this system. Supported by SFB 624.

[1] T. J. Schuerlein et al., JVSTA 12 (1994) 1992. [2] M. Andreasson et al. Synth. Met. 158 (2008) 45

O 35.14 Tue 18:15 Poster B1

Ordered structures of the acceptor molecule TNAP on Au(111) investigated by STM and LEED — •Qinmin Guo, Benjamin Fiedler, Stefan Gärtner, and Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie der Universität Bonn

As a strong electron acceptor 11,11,12,12-tetracyanonaptho-2,6-quinodimethane (TNAP) is attractive for synthesising molecular charge transfer compounds. As a preparatory step we have studied the rich phase diagram of TNAP on the Au(111) surface for varying coverages and temperatures using STM and LEED. We have found at least 4 different structures (α, β, γ, δ) depending on the coverage and post-annealing conditions. α is a 1-dimensional ordered linear structure, and β is the brickwall-like structure reported also in ref. [1]. By post-annealing at 400 K, β can be converted into γ with a T-shaped arrangement of the molecules. The structure δ is only obtained at low temperatures. We will discuss these intermolecular interactions relevant for the structures. In addition, we present first results on binary structures of TNAP with electron donating molecules both on Au(111) and thin epitaxial KCl films on Au(111). This work is supported by SFB 813.

O 35.15 Tue 18:15 Poster B1

Nanostructure formation of hexphenylnitril — •Jörg Meyer[1], Anja Nickel[1], Robin Ohmann[1], Cormac Toher[1], Francesca Moresco[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — [2]Division of IT Convergence Engineering, POSTECH, Pohang 790- 784, Republic Korea

We report the first STM and STS measurements of the asymmetric molecule hexphenylnitril on the Au(111) surface. This molecule consists of six phenyl rings connected via single bonds in the para position (forming a straight line). One side of the molecule is functionalized with a cyano group. At high surface coverages, the molecules exhibit a densely packed parallel structure. At lower surface coverage the molecules tend to adsorb on step edges and adatoms due to their high mobility on the Au(111) surface. Triplets of molecules have also been observed. This triplet structure also verifies the intended asymmetrical structure of the molecule, because bifunctionalized specimens are known to form extended networks with similar triplet structures. To clarify whether the molecules themselves form a self-stabilising nanostructure or just attach to an adatom, we varied the sample temperature during evaporation. With increasing substrate temperature the fraction of triplets among all adsorbates increased. Comparing this to the known increase in the density of adatoms on the Au(111) surface leads to the interpretation of three molecules gathering around single adatoms.

O 35.16 Tue 18:15 Poster B1

Self-assembled Monolayers of Paramagnetic Molecules on Gold revealed by Scanning Tunneling Microscopy — •christian salazar[1], danny baumann[1], ronny schlegel[1], torben hänke[1], jochen lach[2], berthold kersting[2], bernd büchner[1,3], and christian hess[1] — [1]Institute for Solid State Research, IFW Dresden, Germany — [2]Institute für Anorganische Chemie, Universität Leipzig, Germany — [3]Department of Physics, TU Dresden, Germany

We have studied self-assembled monolayers of organic dinickel (II) complexes with an S=2 high paramagnetic state, anchored to a Au(111) surface via thiol groups using STM at room temperature. Our data clearly reveal the dense distribution of 2-4 nm sized objects on the Au surface, which evidences the growth of a closed molecular monolayer. The monolayers, however, do not show long-range order of the individual molecules.

O 35.17 Tue 18:15 Poster B1

STM investigation on the structure formation of the ionic liquid BMP-TFSA on different metal surfaces — •Dorothea Alwast[1,2], Benedikt Uhl[1,2], Florian Buchner[1,2], and R. Jürgen Behm[1] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — [2]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89069 Ulm, Germany

The application of ionic liquids in electrolytes is a promising concept for the improvement of Li-Ion batteries. Therefore, a detailed knowledge of the behavior of ionic liquids on the electrode electrolyte interface is crucial for further development. As a model system, adlayers of 1-butyl-1-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide

(BMP-TFSA) have been investigated by scanning tunneling microscopy (STM). Measurements were carried out under UHV conditions in the submonolayer and monolayer regime, with particular emphasis on the structure formation of the first adsorbate layer. On Ag(111), BMP-TFSA forms a 2D liquid at room temperature, whereas at 100 K an ordered structure is observed on this surface. High-resolution STM images have been acquired and the sub-molecular features will be discussed. Details on structure formation of BMP-TFSA on Ag(111) as well as a comparison to surface structures of BMP-TFSA on Au(111) and Cu(111) surfaces are presented.

O 35.18 Tue 18:15 Poster B1

Combined STM and XPS investigation on the Ethylene Carbonate | Cu(111) interface — •Hanieh Farkhondeh[1,2], Florian Buchner[1,2], Benedikt Uhl[1,2], and Rolf-Jürgen Behm[1,2] — [1]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89069 Ulm, Germany — [2]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Ethylene Carbonate (EC) is an important component in Li-ion battery electrolyte. A molecular understanding of the solid electrolyte interphase (SEI) is crucial to improve the Li-ion battery performance. In this work, the behavior of the EC | Cu(111) interface, as a model system, was investigated at sub-monolayer and monolayer coverages. The adlayers were characterized with STM and XPS under UHV conditions at temperatures between ~100 K and room temperature. With XPS, the intact EC was observed in the multilayer, monolayer and sub-monolayer range around 100 K, where two peaks in the C1s and O1s core level region reflect its stoichiometry. STM data at 100 K show that the molecules aggregate in 2D ordered islands at mono- and sub-monolayer coverages. The contour of these domains strongly changes in time sequence of STM images, which means they are not stable, pointing to weak adsorbate-adsorbate interactions. At room temperature, only noisy features are observed, i.e., EC molecules move too rapidly to be imaged with STM. The co-deposition of Lithium will be conducted in forthcoming experiments.

O 35.19 Tue 18:15 Poster B1

Formation of NTCDA and CuPc (hetero-) organic phases on Ag (111) — •Sonja Schröder, Benjamin Stadtmüller, Christian Wagner, Martin Willenbockel, Christoph Kleimann, Sergey Subach, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and Jülich-Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

The future development of organic devices like solar cells, OLEDs or OFLETs is based on the understanding of the interactions at organic-metal and organic-organic interfaces. In particular, charge transfer and the bonding strength across the interface are important, which in turn depend on the structure and molecular orientation. PTCDA, NTCDA and CuPc are prototypical molecules which have been studied intensively in this context in the last years. Here we report on the adsorption of NTCDA on Ag (111) and on NTCDA-CuPc-heteroorganic films. We present a modified brick wall model for NTCDA on Ag (111) with the molecules oriented perpendicular to the [-1 1 0] direction. This model is based on scanning tunneling microscopy (STM) measurements, pair potential calculations, a LEED I-V analysis and angle resolved photoemission (ARPES) results. Furthermore, we have investigated mixed layers of CuPc and NTCDA at different coverages on the same surface. Three different phases could be identified by SPA-LEED: A NTCDA rich-, a "1:1"- and a CuPc rich phase. The NTCDA- and the CuPc rich phases are commensurate structures. ARPES studies were performed for investigating the electronic properties.

O 35.20 Tue 18:15 Poster B1

Adsorption geometry and chemical structure investigations of organic molecules with atomic force microscopy using functionalized tips — •Bruno Schuler, Leo Gross, Fabian Mohn, Nikolaj Moll, and Gerhard Meyer — IBM Research - Zurich, 8803 Rueschlikon, Switzerland

Atomic force microscopy (AFM) with functionalized tips has proven to achieve intra-molecular contrast due to Pauli repulsion [1]. Crucial factors affecting the image contrast are the tip termination, intramolecular chemical differences and adsorption geometry of the adsorbate. Here we present investigations on all of these three contrast decisive factors. Particularly, we investigated the contrast characteristics of several tip apices (Cl, Br, CO, NO, Xe, Kr) for scanning tunneling microscopy and AFM imaging and developed a new tip preparation method for halogens based on dissociation from molecule precursors [2]. Furthermore, using the high-resolution of the CO tip, we could distinguish bond-order differences in aromatically bonded hydrocarbon molecules [3].

References:

[1] L. Gross, F. Mohn, N. Moll, P. Liljeroth, G. Meyer, Science 325, 1110 (2009)

[2] F. Mohn, B. Schuler, L. Gross, G. Meyer, submitted

[3] L. Gross, F. Mohn, N. Moll, B. Schuler, A. Criado, E. Guitián, D. Peña, A. Gourdon, G. Meyer, Science 337, 1326 (2012)

O 35.21 Tue 18:15 Poster B1

STM and X-ray spectroscopy study on the self-assembly and chemical behavior of orotic acid on close-packed coinage metal surfaces — •Sybille Fischer, Anthoula C. Papageorgiou, Joachim Reichert, Katharina Diller, Francesco Allegretti, Florian Klappenberger, and Johannes V. Barth — Physik Department E20, TU München, James- Franck-Straße, D-85748 Garching

Understanding the self-assembly of small biomolecules including the DNA/RNA bases and related molecules as well as their interaction with metal surfaces is an important step towards the creation of biofunctionalized interfaces. Orotic acid is an important molecule in the *de-novo* synthesis of pyrimidines which include the RNA bases uracil and cytosine. Here we report the results of a multitechnique study investigating the self-assembly and chemical behavior of orotic acid on the Ag(111) and Cu(111) surfaces by means of scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine-structure (NEXAFS). While the molecules assemble in two room-temperature stable structures on the silver surface, we can only find a metastable structure on the copper surface. The XPS study as a function of temperature gives insight in the chemical transformations of the molecule's functional groups, which guide the self-assembly whereas NEXAFS allows us to conclude about the molecular orientation with respect to the surface. Our findings are discussed with reference to the physical and chemical behavior of the related molecule uracil on Ag and Cu.

O 35.22 Tue 18:15 Poster B1

Combined photoemission and STM study of the surface-assisted Ullmann coupling reaction — •Min Chen[1], Jie Xiao[2], Hans-Peter Steinrück[2], Shiyong Wang[3], Weihua Wang[3], Nian Lin[3], and Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg — [2]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg — [3]Department of Physics, Hong Kong University of Science and Technology

The Ullmann reaction, a Cu catalyzed C-C coupling reaction for haloarenes has been used for surface-assisted synthesis two-dimensional covalent nanostructures. Generally, this reaction provides a versatile route to the formation of larger arenes and arene-based extended nanostructures, especially one-dimensional molecular wires and two-dimensional covalent organic networks. In this study, we provide evidence for the Ullmann reaction of 4,4"-Dibromo-p-terphenyl (DBTP) and 1,3,5-Tris(4-bromophenyl)benzene (TBB) on Cu(111) by using X-ray and ultraviolet photoelectron spectroscopy (XPS/UPS) as well as scanning tunneling microscopy (STM). Assisted by Cu atoms from substrate, the C-Br bonds break between 170 and 240 K, and neighboring molecules get linked through intermediate C-Cu-C bonds. Upon further increasing the temperature, the C-Cu-C bonds are transformed into C-C bonds, such that neighboring arene fragments are covalently coupled, while Cu is released from the bridge positions. STM gives insight into the reaction progress on the molecular level. Our results provide an example for a possible strategy towards the bottom-up construction of functional devices based on molecular building blocks.

O 35.23 Tue 18:15 Poster B1

A measurement of the hysteresis loop in force-spectroscopy curves using a tuning-fork atomic force microscope — •Merlin Schmuck, Manfred Lange, Dennis van Voerden, and Rolf Möller — Faculty of Physics, Center of Nanointegration Duisburg-Essen, University of Duisburg- Essen, 47048 Duisburg, Germany

The Analysis of the frequency shift versus distance in noncontact atomic force microscopy (NC-AFM) allows to measure the force gradient between the oscillating tip and a surface (force-spectroscopy measurements). When nonconservative forces act between the tip apex and the surface the oscillation amplitude is damped. The dissipation is caused by bistabilities in the potential energy surface of the tip-sample system, and the process can often be understood as a hysteresis of forces between approach and retraction of the tip. We present the direct measurement of the whole hysteresis loop in force-spectroscopy curves at 77 K on the PTCDA/Ag/Si(111) sqrt(3) x sqrt(3) surface by means of a tuning-fork-based NC-AFM with an oscillation amplitude smaller than the distance range of the hysteresis loop. The hysteresis effect is caused by the making and breaking of a bond between PTCDA molecules on the surface and a PTCDA molecule at the tip. The corresponding energy loss was determined to 0.57 eV by evaluation of the force-distance curves upon approach and retraction. Furthermore, a second dissipation process was identified through the damping of the oscillation while the molecule on the tip is almost in contact with the surface. It reaches a maximum value of about 0.22 eV/cycle.

O 35.24 Tue 18:15 Poster B1

Dynamic studies of octaethylporphyrin Fe(III) chloride — •Dennis van Vörden[1], Manfred Lange[1], Merlin Schmuck[1], Johannes Schaffert[1], Roberto Robles Rodríguez[2], and Rolf Möller[1] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]CSIC-ICN, Universitat Autňnoma de Barcelona 08193 Bellaterra, Barcelona. Spain.

The porphyrin molecule is an archetypal metallorganic complex, which is found in many biochemical molecules like chlorophyll, haemoglobin and cytochrome. Here we investigate submonolayer coverages of octaethylporphyrin Fe(III) chloride (Fe-OEP) on Cu(111) prepared insitu-using a combined LT-scanning tunneling/atomic force microscope.

As a first step, the topography and the orientation of the Fe-OEP molecules is investigated. Two different appearances of the molecule (type A and B) can be found. Type A (unfilled) can be easily manipulated and is mainly found at step edges, while type B (filled) is found individually on the flat terrace.

The comparison of DFT-simulations and STM images reveals, that type A molecules can be identified as dechlorinated (Fe-OEP) while type B are intact octaethylporphyrin Fe(III) chloride molecules. This is further corroborated by the observation that type B molecules can be transformed to type A by an electric pulse which induces a dechlorination of the molecule.

The diffusion of the two types of molecules was studied by comparing different preparation, like evaporating the molecule to the surface at room temperature or direct to the cooled substrate.

O 35.25 Tue 18:15 Poster B1

Scanning Tunneling Microscopy Investigation of CU4Dinit on W(110) — •Dennis Kloczan[1], Sandra Diehl[1], Torsten Methfessel[1], Julia Klanke[2], Eva Rentschler[2], and Hans-Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, D-55128 Mainz, Germany — [2]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Germany

Organic semiconductors are a class of π-conjugated molecules. Due to their property of charge separation by light induced electron transfer they have various applications in solar cells, sensors or switches.

In order to ensure a good adhesion on surfaces, the π-system of the molecule has to be planar. A promising molecule with an increased number of C-rings is Cu4Dinit (copper-tetraazaporphyrin with eight 4-tertbutylphenyl residues).

Using scanning tunneling microscopy (STM) we have imaged Cu4Dinit molecules on a W(110) surface with submolecular resolution at room-temperature. Scanning tunneling spectroscopy (STS) reveals the energetic position of molecular orbitals relative to the Fermi-level of the substrate.

O 35.26 Tue 18:15 Poster B1

Monitoring the ring closure on the ligand of an Fe-Porphyrin molecule — •Gelavizh Ahmadi[1], Valentin Müller[1], Benjamin W. Heinrich[1], José I. Pascual[1,2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]CIC nanoGUNE, 20018 Donostia-San Sebastián, Spain

We used Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) at 4.5K to follow the stepwise transformation of Fe-Octaethylporphyrin (FeOEP) into Fe-Tetrabenzoporphyrin (FeTBP) on Au(111). The annealing to 470 K of submonolayer coverages of FeOEP on Au(111) activates an electrocyclic ring closure of the ethyl groups at the organic ligand. We can identify different intermediate species by STM topography as well as by STS measurements. To double check the proposed reaction scheme, we also produced Fe-TBP by an *in-situ* metalation of free-base TBP on Au(111). This allows for an unambiguous identification of our product.

O 35.27 Tue 18:15 Poster B1

Structural and Electronic Properties of Self-Assembled DCV5T-Me2 Molecules on Au(111): from Sub-Monolayer to Bilayer Coverage — •Zechao Yang[1], Martina Corso[1,2], Chris Lotze[1], Elena Mena-Osteritz[3], Peter Bäuerle[3], Katharina J. Franke[1], and Jose I. Pascual[1,2] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]CIC nanoGune, 20018 Donostia-San Sebastián, Spain — [3]Institute of Organic Chemistry II and Advanced Materials, University of Ulm, Germany

The functionality of organic electronic devices importantly depends on the structural and electronic properties of the metal-molecule interface. Here, we investigate the structural and electronic properties of ultrathin films of substituted oligothiophene molecules on a gold surface using low temperature scanning tunneling microscopy and spectroscopy. The chosen molecule, dicyanovinyl-quinquethiophenes (DCV5T-Me2), is used in organic solar cells. DCV5T-Me2 molecules form either molecular chains, stabilized by intercalated Au atoms, or two-dimensional islands depending on the sub-monolayer coverage. The presence of Au atoms in the chains leads to local modification of their electronic structure: the LUMO of molecules in chains have a low energy unoccupied resonance downshifted due to coordination bonds. In fact, molecules at the chain end shows both the unperturbed state, at the free side, and the down shifted state, at the side in contact with Au atoms with no effect on the other side without coordination bonding. This behavior indicates that one can manipulate molecular orbital alignment within individual molecules by coordination bonding meditation.

O 35.28 Tue 18:15 Poster B1

Electrospray deposition of functionalized platform molecules on Au(111) — Kristof Buchmann[1], •Nadine Hauptmann[1], Christian Hamann[1], Sandra Ulrich[2], Franziska Otte[2], Rainer Herges[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel

The electronic coupling to a metal substrate may affect the electronic and geometric structure of molecules. To preserve the intrinsic properties of molecules it is desirable to decouple the functional groups from the substrate. Partial decoupling can be achieved by supporting a molecule by a molecular platform, conceivably via a spacer group. Using low temperature scanning tunneling microscopy we investigate the triazatriangulenium (TATA) and the trioxotriangulenium (TOTA) platform molecule with various functional groups. The preparation of adlayers of these molecules by thermal sublimation is not feasible due to their thermal instability. We therefore use a home-built electrospray ionization setup for depositing the molecules onto Au(111) in ultrahigh vacuum. The observed tunneling spectra are in good agreement with calculated spectra of the respective gas-phase molecules. This proves the electronic decoupling of the functional groups from the substrate. Financial support by the Deutsche Forschungsgemeinschaft via the SFB 677 is gratefully acknowledged.

O 35.29 Tue 18:15 Poster B1

Comparative study of periodic and non-periodic approaches: Organic π-systems on coinage metals. — •Jaita Banerjee and Reinhold Fink — Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany

We present a comparative study of metal-organic interface properties obtained from DFT calculations based on two different approaches: the periodic slab supercell technique and the cluster ansatz. Such interfaces of aromatic organic molecules with metal substrates form one of the important parts of organic optoelectronic devices. While it is well established that plane waves-pseudopotentials-periodic supercell approaches are reasonable methods to study the geometric and electronic structure of such interfaces, the cluster ansatz has not been much studied. We choose two different π-systems on silver and gold surfaces respectively. The strategy has been to obtain the structure and energetics of each system using the periodic supercell approach, then constructing the metallic clusters from the obtained periodic results. After optimizing the metal clusters, the molecule is placed on its surface and the respective adsorption energies and distances are computed. Our results indicate that while small clusters consisting of two metallic layers form unsuitable systems, clusters with 4 layers begin to show trends as obtained from the periodic calculations. The effect of van der Waals dispersion is also included. Our findings encourage possibilities of using the cluster ansatz to study molecule-metal interfaces since often the size of the organic molecule poses computational challenges in performing a full periodic calculation.

O 35.30 Tue 18:15 Poster B1

Site-specific geometric and electronic relaxation of cobalt-phthalocyanine on Cu(111) — •Christoph Bürker[1], Alexander Gerlach[1], Steffen Duhm[2], Takuya Hosokai[3], Blanka Detlefs[4], Satoshi Kera[5], Nobuo Ueno[5], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, DE — [2]Institute of Functional Nano & Soft Materials, Soochow University, CN — [3]Department of Materials Science and Technology, Iwate University, JP — [4]European Synchrotron Radiation Facility, FR — [5]Graduate School of Advanced Integration Science, Chiba University, JP

We present X-ray standing wave (XSW) and ultraviolet photoelectron spectroscopy (UPS) data of cobalt-phthalocyanine (CoPc) on Cu(111). The XSW technique yields a slightly distorted geometry of the molecule upon adsorption as the cobalt, carbon and nitrogen atoms show different bonding distances (2.50 Å, 2.55 Å, and 2.60 Å, respectively). The relatively strong, chemisorptive interaction between molecule and substrate is confirmed by angle-resolved UPS measurements, which show the appearance of interface states. Hence, these two techniques show a site-specific geometric and electronic relaxation of CoPc on Cu(111). Finally, we compare our data both with theoretical findings for the same system [1] and with ZnPc on Cu(111) [2].

[1] X. Chen and M. Alouani, *Phys. Rev. B* **82**, 094443 (2010)
[2] H. Yamane et al., *Phys. Rev. Lett.* **105**, 046103 (2010)

O 35.31 Tue 18:15 Poster B1

Influence of Bromine groups on the molecular arrangement and adsorption of CuTPPBr$_8$ on Au(111) — •Lars Smykalla[1], Michael Hietschold[1], and Heinrich Lang[2] — [1]Chemnitz University of Technology, Institute of Physics, D-09107 Chemnitz, Germany — [2]Chemnitz University of Technology, Institute of Chemistry, D-09107 Chemnitz, Germany

The bromination of the molecule tetraphenyl-porphyrin leads to a very strong saddle-shape deformation of the macro-cycle and a change of the electronic states. We combine scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), photoemission spectroscopy (PES) and density functional theory (DFT) to thoroughly investigate the molecular arrangement and electronic structure of copper-2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin (CuTPPBr$_8$) on the Au(111) surface. After slight annealing of the sample a well ordered adsorbate structure is observed. Thereby, the molecules are found to be rotated by 90° with respect to their neighbours in a checkerboard-like manner. Upon heating above 300°C the molecular arrangement transforms into a stripe-like structure with two different kinds of molecular appearances, which is due to the debromination of the molecules as could be confirmed by PES. Furthermore, we present a comparison of our results obtained from STS, PES and DFT for the electronic structure of CuTPPBr$_8$ adsorbed on Au(111) and discuss the interaction of the molecules with the substrate.

O 35.32 Tue 18:15 Poster B1

Bistable charge states in the acceptor-donor complex Tetracyanoethylene-Tetrathiafulvalene on Au(111) — •Paul Stoll[1], Janina Ladentin[1], Tobias R. Umbach[1], Christian Lotze[1], Isabel Fernandez Torrente[1], José Ignacio Pascual[1,2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin — [2]CIC nanoGUNE, Donostia-San Sebastián, Spain

The charge state of a molecule has a crucial influence on its physical and chemical properties. Using scanning tunneling microscopy and spectroscopy we investigate the charge-transfer complex consisting of Tetracyanoethylene (TCNE) and Tetrathiafulvalene (TTF) on a Au(111) surface. The two molecules self-assemble in highly ordered mixed islands. The TCNE molecules are found in two different charge states that are identified by the presence or abscence of a Kondo resonance. We observe a current-induced bistability of the two states. The switching yield strongly depends on the bias voltage and varies by orders of magnitude.

O 35.33 Tue 18:15 Poster B1

Simulating Photoelectron Diffraction Measurements of Fe-Porphyrins on Ag(111) — •Michael Greif[1], Tibor Nagy[2], Maksym Soloviov[2], Luca Castiglioni[1], Markus Meuwly[2], Jürg Osterwalder[1], and Matthias Hengsberger[1] — [1]Physik Institut, Universität Zürich, Winterthurerstrasse 190, 8052 Zürich, Schweiz — [2]Department of Chemistry, University of Basel Klingelbergstrasse 80, 4056 Basel, Schweiz

Combing DFT- and force field calculation for iron-porphyrins on an Ag(111) surface not only yields parameters for the equilibrium structure of the molecules adsorbed on the surface, but also information about their dynamics. An experimental means enabling one to visualize structural dynamics are photoelectron diffraction measurements. In these experiments photoelectrons emitted from a molecular atom are coherently scattered by their neighboring atoms. Interference effects thus create a diffraction pattern in the photoelectron signal that is recorded by scanning the half sphere above the sample. From this pattern the structural parameters of the system can be found with a resolution on the sub Angstrom scale. An important analysis tool for those measurements are single scattering cluster (SSC) calculations, which can simulate the experimental outcome. Using Fe-porphyrin as an example we show how time resolved photoelectron diffraction may be used as tool to determine structural dynamics. By combining force-field computations and SSC calculations, it is possible to follow the molecular trajectories while the excited molecule crosses a conical intersection from the excited singlet state to the triplet ground state.

O 35.34 Tue 18:15 Poster B1

Low Temperature Scanning Tunneling Microscopy Study of Co-Phthalocyanine Molecules on Graphene/Ir (111) — •Samuel Bouvron, Philipp Erler, Stefan Ambrus, Elizabeta Cavar, and Mikhail Fonin — Fachbereich Physik, Universität Konstanz

Because of its influence on the electronic and transport properties of a molecule, the interaction between a molecule and a substrate is of crucial importance for possible applications in molecular electronic devices. Furthermore, the adsorption behavior of molecules on surfaces is decisive in a bottom up approach to build molecular electronics. We have investigated the adsorption of cobalt phthalocyanine (CoPc) molecules on epitaxial graphene on Ir(111) by means of low-temperature scanning tunneling microscopy(STM). The small mismatch between graphene and the Ir(111) surface lattice results in a highly ordered hexagonal moiré superstructure with a periodicity of 2.5 nm, making graphene/Ir(111) an interesting template for molecular self-assembly. Here we present the analysis of the nucleation and the early stage growth of CoPc islands on graphene on Ir(111). We report on a subtle competition between intermolecular interactions and substrate-adsorbate interactions for different coverages of CoPc molecules, varying from a submonolayer to a multilayer. Depending on the coverage, we observed different growth modes. At a monolayer coverage, the CoPc molecules arrange in an oblique close-packed structure, whereas at lower coverage a moiré-supported network consisting of ring-like units of six CoPc molecules is observed.

O 35.35 Tue 18:15 Poster B1

Unraveling the adsorption geometry of a 2D metal-organic framework on Cu(111) — Manfred Matena[1], Jonas Björk[2], Kathrin Müller[3], Jorge Lobo-Checa[4], Lutz H. Gade[5], Thomas A. Jung[1], Mats Persson[6], and •Meike Stöhr[3] — [1]University of Basel — [2]University of Linköping — [3]University of Groningen — [4]DIPC, San Sebastian — [5]University of Heidelberg — [6]University of Liverpool

The interest in studying organic nanostructures on surfaces emerges from their prospective applications in nanoscale electronic or optoelectronic devices, in which the spatially addressable functional units are to be assembled on the molecular level. By making use of molecular recognition processes based on non-covalent interactions, well-ordered 1D and 2D molecular structures can be formed on surfaces. Especially, the understanding of the interplay of the underlying intermolecular and molecule substrate interactions are of great research interest since they are responsible for the structure formation and the resulting electronic properties. We report for the perylene derivative DPDI the formation of a nanoporous metal-organic framework (MOF) on Cu(111) upon annealing at 200°C. Scanning tunneling microscopy, low energy electron diffraction, photoemission spectroscopy and X-ray standing wave measurements as well as DFT calculations were carried out to obtain a thorough understanding of the involved interactions and observed (electronic) phenomena. By comparing these findings to similar metal-organic coordination networks common features and differences can be identified.

O 35.36 Tue 18:15 Poster B1

Temperature depending formation of ultrathin FeO(111) films on Ag(111) — •Sören Richard Lindemann, Daniel Bruns, and Joachim Wollschläger — Universität Osnabrück, Fachbereich Physik, Barbarastraße 7, 49076 Osnabrück

Iron oxides are used in various applications in spintronic devices and heterogenous catalysis. Therefore, the preparation and characterisation of thin and ultrathin iron oxide films on different metal substrates stand in the focus of current research. In this study ultrathin iron oxide films were grown on Ag(111) by subsequent deposition of Fe films at room temperature, which is followed by annealing in 10^{-5} mbar O_2 atmosphere at 150°C for 10 minutes to oxidize the submonolayer films. These films were post-deposition annelead at elevated temperatures in Ultra High Vacuum (UHV) to increase the order inside the film lattice. Structure, morphology and chemical composition of the films were investigated before and after this temperature treatment by Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED) and Auger Electron Spectroscopy (AES). Although the diffraction patterns suggest an increase of order at the surface due to annealing, a segregation of silver was observed via AES for temperatures above 300°C. For an annealing temperature of 400°C coexisting FeO(111) and Ag(111) domains at the surface were found with SPA-LEED.

O 35.37 Tue 18:15 Poster B1

Segregation of Ag due to annealing of ultrathin Fe films on Ag(001) — •Christian Otte, Daniel Bruns, Steffen Jentsch, Sören Lindemann, and and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

Thin Fe films are promising candidates for application in spintronic devices due to their electric and magnetic properties. In this work, ultrathin Fe films grown at room temperature on Ag(001) were post-deposition annealed in Ultra High Vacuum (UHV) at 250°C. This was monitored via X-Ray Photoelectron Spectroscopy (XPS) and Auger Electron Spectroscopy (AES). The surface structure and morphology was studied before and after annealing in UHV by Scanning Tunneling Microscopy (STM) and Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED). The as-deposited Fe forms column shaped islands. Annealing in UHV at 250°C leads to a strong change in surface structure and morphology accompanied by surface segregation of Ag. While SPA-LEED shows an additional $(\sqrt{2} \times \sqrt{2})$R45° superstructure after annealing, STM reveals large, flat Ag(001) terraces without any superstructures on them. Strongly three dimensional structures are likely to contain part of the deposited Fe. Nevertheless the XPS results suggest that most of the Fe has to be buried underneath the segregated Ag. This assumption is supported by energetic considerations comparing surface free energies of Fe(001) and Ag(001).

O 35.38 Tue 18:15 Poster B1

Epitaxial growth of Fe on Ag(001) revisited: Film stress measurements as a monitor of interface formation — •Kenia N. Fischer[1,2], Dirk Sander[1], Andre A. Pasa[2], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]LFFS, Universidade Federal de Santa Catarina , Florianópolis, Brazil

The growth of Fe on Ag(001) has created a lot of controversy regarding the growth mode in the first monolayers [1]. Early studies reported layer-by-layer growth up to 3 layers, whereas careful LEED studies [1] and EXAFS studies [2] ruled that out. Instead, surface alloying and a rough surface morphology were proposed for the first layers of Fe. Our measurements of Fe-induced film stress on Ag(001) show a nonmonotonic change of stress in the first layers. A surprisingly large tensile stress of +7.3 GPa is observed for the first 0.5 ML Fe deposition, which is followed by a compressive stress of -0.73 GPa from 0.5 to 1.5 ML. Then a tensile stress sets in, which leads to an average film stress of +2 GPa in a 10 ML Fe film. The magnitude of stress and its change of sign come as a surprise. The epitaxial misfit of +0.8 % leads to a calculated misfit stress of +1.7 GPa, in contrast to our observations. The observed stress variations in the monolayer range cannot be ascribed to simple layer-by-layer growth of an epitaxially strained Fe film. Rather, intermixing and surface stress change of the substrate upon film deposition need to be considered [3]. [1] Li et al., Phys. Rev. B 42(1990)9195. [2] Hahlin et al, Phys. Rev. B 73(2006)134423. [3] Mahesh et al., Phys. Rev. B 68(2003)045416.

O 35.39 Tue 18:15 Poster B1

Thickness-dependent growth study of Bi on Au(111) — •Jeannette Kemmer, Jens Kügel, Pin-Jui Hsu, and Matthias Bode — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg

We have performed a growth study of ultra-thin Bi films on a Au(111) substrate. Upon Bi growth at room temperature the film morphology was determined with a home-built low-temperature Scanning Tunneling Microscope (STM). Within the thickness range between submonolayer coverage up to 3 atomic layers (AL) topographic images show various surface reconstructions, including the so-called (6×6)-structure at 0.5 AL which has been reported previously [1] and resembles the well-known Si(111)-7×7 reconstruction. In addition, our data show extended areas with one-dimensional superstructures, which are preliminary assigned to $2\sqrt{3} \times 2\sqrt{3}$ R30°- and a larger $10\sqrt{3} \times 10\sqrt{3}$ R30°- unit cells.

[1] J.H. Jeon *et al.*, Surf. Sci. 603, 145 (2009).

O 35.40 Tue 18:15 Poster B1

Adsorbate-induced segregation: a quantitative first-principles study for $C/Pt_{25}Rh_{75}(100)$ — •Tobias C. Kerscher[1], Wolfgang Landgraf[2], David Reith[3], Raimund Podloucky[3], and Stefan Müller[1] — [1]TU Hamburg-Harburg — [2]Universität Erlangen-Nürnberg — [3]Universität Wien

For catalytic surfaces, such as Pt-Rh, it is essential to understand the change in the segregation profile due to the presence of adsorbates. Our prior first-principles studies of adsorbate-induced segregation in $C/Pt_{25}Rh_{75}(100)$ have shown that, compared to the clean surface, a small amount of carbon impurities suffices to substantially decrease the Pt concentration in the top layer of the substrate. We corroborated this view at $T = 0$ K by DFT and the cluster expansion (CE).

Now, we have improved the CE to increase its accuracy for the complex interactions between several substrate and adsorbate layers. This enables us to quantitatively predict the T-dependent, layer-by-layer segregation profile of the substrate subject to C-contamination [1]. Our CE code UNCLE [2] uses a bisection of the simulation lattice into separate subsystems—already discussed during the last years—in combination with a new averaging procedure [3]. We discuss the coupling of the substrate and adsorbate layers in the CE, the $T = 0$ K stability diagram, and the T-dependent segregation profile for different C-contaminations. (Supported by DFG.)

[1] T. C. Kerscher *et al.*, Phys. Rev. B **86**, 195420 (2012)

[2] D. Lerch *et al.*, Modelling Simul. Mater. Sci. Eng. **17** (2009), 055003

[3] D. Reith *et al.*, Phys. Rev. B **86**, 020201(R) (2012)

O 35.41 Tue 18:15 Poster B1

Preparation of PtCu core-shell model catalyst electrodes — •Albert K. Engstfeld, Andreas Bensch, Christoph K. Jung, Regine Weiss, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Core shell particles consisting of a metal A rich shell and a bi- or multialloy core show a different catalytic activity compared to pure metal particles. An interesting example are Pt enclosed alloy particles containing Cu, Co and Pt, which have a much better activity towards the electrocatalytic oxygen reduction than pure Pt.

We will describe on the one hand the preparation of PtCu core on Ru(0001) and on the other hand the preparation of a Pt shell on these alloy surfaces, which reflects a model catalysts for core shell particles. The surfaces were investigated by scanning tunneling microscopy under ultra high vacuum conditions. The formation of PtCu monolayer alloys on Ru(0001), is found to be kinetically hindered, due to the strong binding of Pt to the Ru substrate. This limitation can be overcome, however, by careful selection of the experimental conditions (annealing time, deposition sequence ...).

Depositing Pt on Cu sub-monolayer films on Ru(0001), we find a strong tendency for a place exchange between Pt and the Cu upon room temperature deposition of Pt. This allows the fabrication of 2D PtCu model cores with at least 20 % Pt, which can be used as substrate for subsequent Pt deposition. We will discuss the homogeneity of the system after both preparation steps in view of potential use as model catalyst for further electrochemical/-catalytic investigations.

O 35.42 Tue 18:15 Poster B1

Improving the Quality of SiC Surfaces by Precise Definition of H2-Etching Parameters — •Tobias Denig and Ulrich Starke — Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart Germany

SiC is a material of great technical interest because it offers an attractive combination of chemical robustness and excellent thermal and electrical properties. However, in order to make use of these characteristics one needs a well-behaved, passivated surface. This has led to the prevalence of a H2 etching step in SiC processing, as it simultaneously removes surface damage (e.g., polishing scratches), reduces the defect density, and leaves behind an "atomically-flat," H-terminated terraced surface. In the ideal limit, such steps should be one SiC bilayer (0,25 nm) thick. A common occurrence in such etching is for two or more steps to bunch, producing steps of one or several unit cell heights. The end result is a mixture of step heights, producing a sub-optimal surface for further work. However, one unit cell height should be a natural step size due to the particular stacking order in SiC polytypes. Various etch parameters (gas flowrate, T, and p) can influence the amount of step bunching. We have performed parameterization studies aimed at limiting this process such that only steps of (single) unit cell height emerge. All samples used in these studies underwent a modified RCA clean prior to being etched. The results of varying the processing conditions as well as using Ar or H2 as the cooling gas were examined using XPS, LEED, and AFM.

O 35.43 Tue 18:15 Poster B1

UV laser supported oxide removal from Si seed layers for thin-film Si solar cells — •Roman Bansen, Robert Heimburger, Franziska Schütte, Thomas Teubner, and Torsten Boeck — Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

To achieve low temperature deposition of crystalline Si on glass for photovoltaic applications, a two-step process has been developed at Leibniz Institute for Crystal Growth. In the first step, amorphous Si films are crystallized at temperatures around 300°C by means of metal-induced crystallization. In the second step, they are used as templates for further Si deposition by steady-state solution growth. Between the two steps, during handling in high vacuum conditions, the templates form a thin layer of Si oxide. This is a major obstacle for the second step, as it hinders epitaxial growth. Conventionally, oxide desorption from Si is achieved by an annealing step above 800°C, a method which cannot be applied to glass substrates. We discuss several approaches involving in situ treatment of oxidized surfaces with UV laser irradiation in highly pure H2 atmosphere. One approach is the removal of Si oxide by ablation. Another approach involves the lowering of the oxide desorption temperature during simultaneous UV laser irradiation below the ablation threshold.

O 35.44 Tue 18:15 Poster B1

And Now For Something Completely Different: Au Induced Faceting of Si(0 8 15) — •Christian Witt, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — Faculty for Physics and Center for Nanointegration CENIDE,University Duisburg-Essen Lotharstrasse 1, 47057 Duisburg

Au and Ag are known to induce faceting on many vicinal Si surfaces. Until now, studies have focused on the faceting kinetics in one dimensional systems, where a distinct step orientation of the vicinal substrate was transformed into a faceted surface with straight step edges and a zigzag cross section. Here, we show similar experiments on a surface that exhibits two faceting directions during depositionof Au at elevated temperatures. Si(0 8 15) is a vicinal Si(0 1 2) surface with a miscut of 1.51° towards (0 2 -1). We observed the faceting kinetics of this surface by low energy electron microscopy and low energy electron diffraction. During Au adsorbtion the surface initially forms one dimensional facets. This is followed by a second faceting transformation to form an Escher-like "checkered" pattern. After completed faceting we find three different types of facets with typical facet sizes of few hundred nm. The facets angles relative to the surface normal were determined by in-situ reciprocal space mapping and independently confirmed by ex-situ AFM measurements. The Au induced faceting transformation of the (0 8 15)face of Si produces two well-ordered facets while leaving the third facet a stepped area with characteristic convex and concave areas. [1] Phys. Rev. Lett. 86 (2001) 5088; [2] J. Phys.: Cond. Matter 18 (2006) 1; [3] Surf. Rev. & Lett. 5 (1998) 1164

O 35.45 Tue 18:15 Poster B1

Bi$_2$Se$_3$ films on Si(111): Growth optimization and in-situ SPA-LEED measurements — •Michael Vyshnepolsky, Claudius Klein, Anja Hanisch-Blicharski, and Michael Horn-von Hoegen — Fakultät für Physik und Center for Nanointegration CENIDE, Universität Duisburg-Essen, Lotharstr. 1, D-47057 Duisburg, Germany

Employing high resolution spot profile analysis low energy electron diffraction (SPA-LEED), atomic force microscopy (AFM) and x-ray diffraction (XRD) we studied the growth of Bi$_2$Se$_3$ on Si(111). The films were prepared by thermal co- deposition of Se and Bi with a flux ratio of 10:1 at temperatures between 200 and 250 °C. The strain relaxation during the growth of the first quintuple layers was measured in-situ during deposition by tracking the (01)-spot position with SPA-LEED. At a thickness of 6 nm the Bi$_2$Se$_3$ film exhibits a lateral lattice parameter of 4.02 Å. The decrease of the spot width of the (00)-spot reflects that the crystal quality improves by post-growth annealing up to temperatures of 350 °C. This is also confirmed in the AFM measurements, where remaining Se wires disappear with higher annealing temperature. XRD measurements of Bi$_2$Se$_3$ films with thickness of 70-80 nm verifies the high film quality and also confirms the vertical lattice parameter of 28.63 Å.

O 35.46 Tue 18:15 Poster B1

Cd-content analysis of capped and uncapped CdSe quantum dots on ZnSe by Raman spectroscopy — •Utz Bass, Constantin Weiler, Jean Geurts, Alex Frey, Suddhasatta Mahapatra, and Karl Brunner — Universität Würzburg, Physikalisches Institut, Am Hubland, 97074 Würzburg

Quantum Dots (QD) offer the intriguing opportunity to study fundamental low-dimensional physics and are simultaneously employed in optoelectronic applications. Wide band gap II-VI semiconductor QD are promising candidates to extend the applications to the visible energy regime. The self-assembly of the CdSe/ZnSe QD system is driven by the large lattice mismatch. The strain relaxation mechanism consists of dot formation together with intermixing of Cd and Zn. In this study we focus on the Cd-content analysis of CdSe QDs embedded in or on top of ZnSe. CdSe QD sample series with different nominal CdSe thickness values from various MBE growth procedures are investigated by Raman spectroscopy (RS), accompanied by photoluminescence (PL). Also for uncapped QDs with quenched PL, RS enables the Cd-concentration analysis and thus allows the in-situ study of QDs. The comparison of the capped and uncapped QD results shows that the overgrowth of the QDs with the capping ZnSe layer induces a considerable additional intermixing. This susceptibility for intermixing during overgrowth explains, why on overgrown QDs the observed Cd-content essentially only depends on the nominal CdSe-thickness, although AFM-studies of uncapped QDs showed clear morphology differences for the different growth procedures.

O 35.47 Tue 18:15 Poster B1

Preparation of GaP/Si(111) quasi-substrates for III-V nanowire solar cells — •Weihong Zhao[1,2], Agnieszka Paszuk[1,2], Matthias Steidl[1,2], Sebastian Brückner[1,2], Anja Dobrich[2], Johannes Luczak[2], Peter Kleinschmidt[1,3], Henning Döscher[1,2], and Thomas Hannappel[1,2,3] — [1]Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98684 Ilmenau — [2]Helmholtz-Zentrum Berlin, Institut für Solare Brennstoffe und Energiespeichermaterialien, D14109 Berlin — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D99099 Erfurt

Meeting the demands of high-quality-low-cost photovoltaics, III-V nanowires grown on Si(111) substrates present a promising new solar cell concept. GaP buffer layer can be grown almost lattice matched on Si(111) substrates. Succesful nanowire growth requires atomically smooth/flat GaP(111)B surfaces. Therefore a suitable Si(111) surface preparation is crucial.We used a metal organic vapor phase epitaxy (MOVPE) reactor to prepare GaP/Si (111) quasi-substrates . A contamination-free transfer system enables us to assess the MOVPE prepared surfaces with numerous UHV based surface science tools. A dedicated wet-chemical pretreatment is crucial to obtain atomically flat Si(111) surfaces, and high temperature annealing removed all contamination. It is shown that our preparation in a hydrogen ambient results in a monohydride terminated (1x1)-reconstructed Si(111) surface. Since LEED can identify the different GaP(111)A and B surfaces we found that the Si surface termination influences the polarity of GaP films grown on Si(111) substrates.

O 35.48 Tue 18:15 Poster B1

Characterization of Carbon-Nitrogen-codoped TiO$_2$ with XPS - influence of annealing temperature — •Julian Fischer, Christian Gebauer, Thomas Diemant, Joachim Bansmann, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

TiO$_2$ has been used for photo-electrochemical applications, e.g., in water splitting. However, the large band gap of the material limits its efficiency in the optical regime. Doping of TiO_2 with carbon and nitrogen is expected to reduce the band gap of the material by inducing defect states (acceptor and donor states) in the band gap and increase the electrical conductivity [1].

The samples used in this study were prepared via a sol-gel process [2] using urea (nitrogen donor source) and tetrabutyl titanate as a precursor. The materials were finally calcined in a temperature regime ranging from 175°C to 400°C (3h) and afterwards measured by XPS to characterize their chemical composition; special attention was paid to the inclusion of C and N species into the TiO_2 lattice. The doping of the material can be traced back to two different species: (i) carbon doping is attributed to a C-O species and (ii) nitrogen doping to a Ti-O-N species.

[1] D. Chen et. al., Ind. Eng. Chem. Res. 2007, 46, 2741.

[2] H. Sun et. al., Ind. Eng. Chem. Res. 2006, 45, 4971.

O 35.49 Tue 18:15 Poster B1

XPS analysis of Carbon-Nitrogen codoped TiO_2 - influence of pH and codoped Boron — •Fabian Argast[1], Christian Gebauer[1], Thomas Diemant[1], Joachim Bansmann[1], Maximilian Wassner[2], Nicola Hüsing[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm — [2]Paris-Lodron-University Salzburg, A-5020 Salzburg

TiO_2 has been used for photo-electrochemical applications, e.g., in water splitting. However, undesired recombination of photoexcited carriers and a high band gap of TiO_2 limit its practical application and efficiency. Doping of TiO_2 with boron, carbon and nitrogen is expected to reduce the band gap of the material by inducing defect states in the band gap and increase the photocatalytic activity for light absorption into the visible region [1].

The samples were prepared via a sol-gel process using tetrabutyl titanate as a precursor. In a first approach, tetrabutylammonium hydroxide or tetrabutylammonium nitrate were used as donor sources for C and N. Furthermore, the possible influence of different pH environments were investigated. Next, urea (N and C donor) as well as boric acid were used as co-dopands with the same precursor. The samples were calcined at a temperature regime ranging from of 175°C to 400°C (3h) and afterwards measured by XPS to characterize their chemical composition, especially the inclusion of B, C and N species into the TiO_2 lattice.

[1] D. Chen et. al., Ind. Eng. Chem. Res. 2007, 46, 2741.

O 35.50 Tue 18:15 Poster B1

Density functional calculations for $SrTiO_3$(001) and Fe/$SrTiO_3$ — •Brahim Belhadji and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel

Magnetoelectric coupling at, e.g., the interface of magnetic *d*-metals and $BaTiO_3$ [1] has attracted a lot of interest also in view of applications, like sensors. The magnetization of thin Fe-films on $BaTiO_3$ or $SrTiO_3$ has been shown to depend even qualitatively on the number of Fe-layers [2]. The comparison of *d*-metals on $BaTiO_3$ and $SrTiO_3$ will open up the opportunity to compare different contributions to the magnetoelectric coupling mechanism at such interfaces. As a first step we have studied the clean (001) surface of $SrTiO_3$. The electronic structure is calculated using VASP code. We focus on the experimentally observed $\sqrt{5} \times \sqrt{5}$ reconstruction and compare the Sr-adatom model proposed in [3] and the surface atomic geometry proposed in [4] (and two simple (1× 1) surface terminations as a reference). Scanning tunneling microscopy images are simulated within the Tersoff-Hamann model for both surfaces and various voltages. Furthermore we report first calculations for a single up to few monolayers of Fe on the (001) surface of $SrTiO_3$ and compare to previous work [2]. This lays the basis for a future study of magnetoelectric coupling mechanisms in case of thin *d*-metal films on these titanates.

[1] Chun-Gang Duan *et al.* PRL **97** (047201)(2006).

[2] M. Fechner *et al.* PRB **78**, 212406 (2008).

[3] T. Kubo *et al.* PRL **86**, 1801 (2001).

[4] D. M. Kienzle *et al.* PRL **106**, 176102 (2011).

O 35.51 Tue 18:15 Poster B1

Carbon monoxide on ZnO(10-10) Surface: An Infrared Reflection Absorption Spectroscopy study — •Maria Buchholz, Alexei Nefedov, and Christof Wöll — Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

One of the most important oxides is zinc oxide (ZnO) according to its semiconducting and optical properties. Numerous IR investigations of oxide powders have been reported[1], but however, an unambiguous assignment of the features in the complex powder IR spectra recorded for molecules bound to the oxide powder particle is only possible on the basis of data recorded for well-defined reference systems, e.g. surfaces of single crystals.

The different surfaces of ZnO single crystals are used for investigations, both polar Zn- or O-terminated ZnO {0001} and mixed-terminated ZnO(10-10) surface, which is the dominating surface for ZnO powder particles and energetically most favorable. In this study we investigated adsorption of carbon monoxide on ZnO(10-10) surface, which is model system for many reactions in catalysis. Our results give us the information about the orientation of CO on the surface, which is very important for the reaction mechanism[2].

M. Buchholz gratefully acknowledges the financial support from the Helmholtz Research School "Energy-Related Catalysis".

[1]H. Noei, C. Wöll, M. Muhler, Y. M. Wang, Appl Catal a-Gen 2011, 391, 31-35. [2]M. C. Xu, H. Noei, K. Fink, M. Muhler, Y. M. Wang, C. Wöll, Angew Chem Int Edit 2012, 51, 4731-4734.

O 35.52 Tue 18:15 Poster B1

The role of the anchoring ligand BINA to the binding of the N3 dye on TiO2 anatase (101) — •C. Dette[1], C. S. Kley[1], S. Jung[1], G. Rinke[1], J. Cechal[1], S. Rauschenbach[1], C. Patrick[3], F. Giustino[3], S. Stepanow[1], and K. Kern[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; — [3]University of Oxford, Department of Materials, Oxford, United Kingdom

The rapid increase of power consumption demands new sustainable and low-cost energy sources like dye-sensitized solar cells (DSSCs) in which a layer of dyes is adsorbed on a mesoporous TiO2 film. Even though a lot of work has been dedicated to DSSCs, the adsorption and electronic properties of a single dye molecule and the TiO2 surface remain unclear. Since the adsorption of the dye molecules is determined by the anchoring ligand group, the adsorption geometry and electronic properties of these ligand groups are of crucial importance. Here, we study the properties of N3 dye anchoring ligand BINA (bi-isonicotinic acid) on the TiO2 anatase (101) surface by means of scanning tunneling microscopy and spectroscopy methods in ultra high vacuum. We present different adsorption geometries consistent with first-principle density functional theory based calculations and the corresponding electronic properties. In addition, we discuss the influence of the different binding geometries of the ligand BINA to the N3 dye molecule which shows variable adsorption geometries in contrast to theoretical predictions suggesting only one specific thermodynamically stable N3 adsorption configuration.

O 35.53 Tue 18:15 Poster B1

Optical spectroscopy of PTCDA molecules on a KCl (100) surface in the limit of low coverages: site selection and diffusion — Alexander Paulheim, Mathias Müller, Christian Marquardt, and •Moritz Sokolowski — Institute for Physical Chemistry, University of Bonn, Wegelerstraße 12, 53115 Bonn, Germany

We use optical spectroscopy as a tool to study aggregation and structural site transitions of molecules in the limit of isolated entities on a surface. For this purpose we performed optical spectroscopy on the model molecule perylene-3,4,9,10-tetracarboxyl acid dianhydride (PTCDA) for very low coverages (below 1% of a monolayer) on thin (100) oriented KCl films, epitaxially grown on a Ag(100) surface. The structural and optical properties were investigated by SPA-LEED and by fluorescence and FL excitation spectroscopy, respectively. Two different states of PTCDA molecules can be distinguished: an initial state which is observed directly after deposition onto the cold (20 K) sample, and a final state which is found after thermal annealing or intensive optical excitation. The spectrum of the final state is blue-shifted with respect to that of the initial state by 130 cm^{-1} and exhibits a smaller FWHM due to reduced inhomogeneous site broadening. We explain this by a thermally or optically induced diffusion of the PTCDA molecules from initial terrace sites to energetically favored step edge sites as seen by Karacuban et al. [1] with STM. Polarization dependent spectroscopy reveals the same azimuthal orientation of the molecules on both adsorption sites.

[1] H. Karacuban et al., Nanotechnology 2011, 22, 295305.

O 35.54 Tue 18:15 Poster B1

DFT+D Van-der-Waals C_6 coefficients for ionic crystals — •Steffen Seiler and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

Previous studies have shown that Grimme's dispersion correction to DFT [1] leads to an overestimation of the binding energy of molecules on ionic surfaces. The reason is that in the Grimme D2 scheme no distinction is made between Van-der-Waals C_6 coefficients for neutral and charged species of the same element, although they clearly possess different polarizabilities. We propose a simple scheme for adjusting the C_6 coefficients of the cations in ionic crystals which is based on the static polarizability. Thin films are exposed to an external electric field and the film polarizability is determined by linear regression of the induced dipole moment. The method has been applied to magnesium oxide and hydroxide and we obtained very similar C_6 values for the Mg cations as recently proposed by the Grimme group based on TDDFT calculations [2]. To demonstrate the impact of the modified Van-der-Waals correction, calculated binding curves for the interaction of different small molecules (CH_4, H_2O and $SiMe(OH)_3$) with magnesium oxide and hydroxide model clusters will be shown and the results will be compared to MP2 benchmark calculations.

[1] S. Grimme, *J. Comp. Chem.* **27**, 1787 (2006).
[2] S. Ehrlich et al.,*Chem. Phys. Chem.* **12**, 3414 (2011).

O 35.55 Tue 18:15 Poster B1

Self-assembly of cobalt phthalocyanine molecules on ultrathin CoO(111) films on Ir(100) — •Tobias Schmitt, Pascal Ferstl, Lutz Hammer, and M. Alexander Schneider — LS f. Festkörperphysik, Uni. Erlangen, Germany

We investigated the adsorption of cobalt phthalocyanine (CoPc) molecules on a bilayer of CoO(111) on Ir(100)[1] by low-temperature scanning tunneling microscopy in UHV. CoPc molecules prefer to lie flat on that surface with the Co-Ion centered above oxygen atoms. The rotational orientation of the molecules is determined by the interaction of N-atoms of the macrocycle with the underlying Co-atoms and between π-electrons and the oxygen atoms of the substrate. This leads to adsorption geometries which are dominated by molecule-substrate interaction similar to those found on TiO_2[2]. At higher coverage (0,7 ML) one-dimensional chains with a core-core distance of 1.3 nm are formed while the molecular adsorption site and orientation stay the same. This points to a short-ranged intermolecular interaction, that governs the self-assembly. Only at a coverage of $\simeq$1 ML the CoPcs rotate to decrease the C-N..H hydrogen bond length. We discuss these findings also in the light of the dense structures formed on metal surfaces [3].

[1] C. Tröppner, et al., Phys. Rev. B, in press
[2] Y. Wang, et al., J. Phys. Chem. B 2006, 110, 17960
[3] Y. Wang, et al., J. Am. Chem. Soc. 2009, 131, 10400

O 35.56 Tue 18:15 Poster B1

Interaction of N_2 with the NaCl(100) surface: a combined LEED and DFT-D study — •Jochen Vogt — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The NaCl(100) surface is one of the laboratory model systems to study the elementary processes of the heterogeneous chemistry of the earth's atmosphere [1], whose main constituent is N_2. Detailed experimental results on the adsorption geometry and the binding energy of the system N_2/NaCl(100) have been lacking so far. Low-energy electron diffraction experiments, using a microchannelplate-LEED optics and nanoampere beam currents, reveal a (1×1) symmetry of the first layer N_2 physisorbed on NaCl(100) at temperatures between 20 K and 45 K [2]. This contribution compares the results of a quantitative LEED structure analysis with the minimum energy structure predicted by dispersion-corrected DFT calculations. The experimental adsorption energy including lateral interactions, as determined experimentally within a Fowler-Guggenheim kinetic model of adsorption, are compared to the corresponding predictions from DFT-D. Differences between experiment and theory are discussed, along with possible sources of error.

[1] J. C. Hemminger, Int. Rev. Phys. Chem. 18 (1999), 387
[2] J. Vogt, J. Chem. Phys. 137 (2012), 174705

O 35.57 Tue 18:15 Poster B1

Adsorption of small molecules on ZnO surfaces — •Jakub Goclon and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

Despite much experimental effort the co-adsorption of H_2 and CO on ZnO surfaces, which is of considerable interest in the context of methanol synthesis from syngas, is not well understood. We performed DFT calculations on CO interaction with clean and partially hydrogenated flat ZnO($10\bar{1}0$) as well as stepped ($10\bar{1}1$) and ($20\bar{2}1$) surfaces, including both Zn and O terminations. For the thermodynamically most stable configurations we find a very good agreement for the characteristic Zn-H and O-H vibrational frequencies with the experimental IR signatures.

The majority of catalysts are deactivated even by small amounts of sulfur-containing molecules that are present as impurities in the feed gas. Under reaction conditions those compounds are hydrogenated to form H_2S, for which ZnO is a very efficient low-temperature adsorbent [1]. In the second part of this work, we examined different surface forms of H_2S on the ZnO($10\bar{1}0$) surface and determined the most stable configurations as function of the H_2S chemical potential [2]. In addition, results on sulfur incorporation into the ZnO surface will be shown.

[1] J.M. Davidson, C.H. Lawrie, K. Sohail, *Ind. Eng. Chem. Res.* **34**, 2981 (1995).
[2] J. Goclon, B. Meyer, submitted to PCCP.

O 35.58 Tue 18:15 Poster B1

Interaction of N2O with TiO2 and ZnO Surfaces Studied by IR Spectroscopy — •Max Kauer[1], Heshmat Noei[2], Martin Muhler[2], Karina Morgenstern[1], and Yuemin Wang[1,2] — [1]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, D-44780 Bochum — [2]Lehrstuhl für Technische Chemie, Ruhr-Universität Bochum, D-44780 Bochum

Metal oxides have recently attracted enormous attention because of their important applications in a variety of fields such as catalysis, chemical sensors, solar cells, and electronic devices. We investigated the adsorption of N2O on rutile TiO2(110) and ZnO(10-10) single crystal surfaces by UHV-FTIR spectroscopy. The high-quality IR data demonstrates that exposing both, TiO2 and ZnO to N2O at 120 K leads to molecular adsorption in a linear configuration. However, the binding energy of N2O on ZnO(10-10) is much higher than that on TiO2(110). It was found that N2O is bound to surface Ti4+ ions on TiO2(110) via its O-end, while it prefers to adsorb via its N-end at surface Zn2+ ions on ZnO(10-10). Our results reveal that the N2O adsorption on oxide surfaces is structure-sensitive. The experimental data will be further discussed based on theoretical calculations.

O 35.59 Tue 18:15 Poster B1

Proton distribution and transfer at the titanate/water solid-liquid interface — •Christina Ebensperger, Christof Jäger, and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

Layered sodium titanates show a rich structural behavior in aqueous environments. Sodium ions dissolve and the surfaces become protonated. In acid solution single titanate layers can detach and nanoscrolls are formed. To obtain a more detailed understanding of the surface protonation we performed DFT calculations and Car-Parinello molecular dynamics simulations for sodium titanate surfaces in contact with vacuum, a monolayer of water molecules and a liquid water reservoir. We find that the energetical hierarchy of preferred protonation sites and the proton distribution depend on the environment and change from vacuum to thin water films and the solid-liquid interface. A full explicit treatment of the liquid surrounding is thus mandatory for obtaining realistic surface structures. In the CPMD simulations we observe water-mediated transfers of surface protons between different adsorption sites. In rare cases spontaneous de-protonation events of the surface occur, which may explain the negative surface charge observed in experiments.

O 35.60 Tue 18:15 Poster B1

Investigation of the MgO absorbate and the MgO/Fe on GaAs(001) surface by means of XPS and XPD — •Dominique Handschak[1,2], Tobias Lühr[1,2], Frank Schönbohm[1,2], Christoph Keutner[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund, Germany

We report on a combined high-resolution photoemission (XPS) and photoelectron diffraction (XPD) investigation of magnesium oxide on

Fe. Magnesium oxide is an appliciable insulator in magnetic tunnel junctions (MTJ) based on the tunnel magnetoresistance (TMR)[1]. TMR-components are also of interest in the research of magnetoresistive random access memories (MRAM) [2,3,4]. In this study we report on the crystalline properties of the MgO adsorbate and the MgO/Fe interface. The results of the diffraction patterns revealed an interface with oxidized iron layers and partially shifted magnesium layers in a halite structure.

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O 35.61 Tue 18:15 Poster B1

Themal stability of thin HfO_2 films and structure determination of $HfSi_2$ islands on Si(110) surfaces. — •Frank Schönbohm[1,2], Tobias Lühr[1], Dominique Handshak[1], Lothar Brosda[1], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

Thin SiO_2 gate dielectrics in MOSFETs lose their efficiency because of an increasing leakage current when their thickness is reduced below 2 nm. A possible way omitting this problem is substituting the SiO_2 gate dielectric by another material with a higher dielectric constant. Perspective replacement candidates among the so called *high-k* materials are the oxides of hafnium and zirconium. However, their thermal stability at elevated temperatures is important during the production process. Due to the recent interest in the Si(110) surface orientation we studied thin HfO_2 films on Si(110). Photoelectron spectra of Si 2p, Hf 4f, and O 2s signal as a function of annealing temperature were recorded in oder to investigate the thermal stability of the system. The thin HfO_2 films are stable up to 730°C and form $HfSi_2$ under further annealing at 770°C. Further investigations showed that $HfSi_2$ is arranged in islands at the surface. The $HfSi_2$ islands were investigated by means of photoelectron diffraction (XPD) in order to examine their structure. We present the XPD diffraction pattern and the structure model of the $HfSi_2$ islands which was obtained by computer simulations.

O 35.62 Tue 18:15 Poster B1

Magnetic properties of ultrathin iron oxide films on MgO(001), grown in oxygen atmosphere — •Nico Pathé[1], Tobias Schemme[1], Timo Kuschel[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück — [2]Fakultät für Physik, Universität Bielefeld, Universitätsstrasse 25, 33615 Bielefeld

Due to its characteristics in Giant Magneto Resistance (GMR), iron oxides can be used in magnetoresistive memory devices. In this work, ultrathin iron oxide films were reactively grown on MgO(001) at 250°C. Therefore, the oxygen partial pressure was increased from $5 \cdot 10^{-7}$ mbar to $5 \cdot 10^{-4}$ mbar. Since this has a strong influence on the stoichiometry, the films were charakterized by X-Rax Photoelectron Spectroscopy (XPS). The surface structures were studied by Low Energy Electron Diffraction (LEED) and the magnetic properties of the films were investigated via Magneto-Optic Kerr Effect (MOKE). The XPS data shows that there's still elemental Fe at the surface after preparation in $5 \cdot 10^{-7}$ mbar O_2. For oxygen partial pressures of $5 \cdot 10^{-6}$ mbar and above only Fe^{2+} and Fe^{3+} ions can be found on the surface. Just between $5 \cdot 10^{-6}$ mbar and $5 \cdot 10^{-5}$ mbar Fe_3O_4 is formed at the surface. This is confirmed by LEED measurements, which show the expected $(\sqrt{2} \times \sqrt{2})R45°$ superstructure for these films. MOKE reveals, that the films grown at an oxygen partial pressure of $5 \cdot 10^{-7}$ mbar and $5 \cdot 10^{-5}$ mbar have a fourfold magnetic anisotropy. The easy axes are aligned in Fe_3O_4 [110] direction.

O 35.63 Tue 18:15 Poster B1

Epitaxial growth of NaCl on thin KCl(100) films on Ag(100) studied by SPA-LEED — •Christian Marquardt, Alexander Paulheim, and Moritz Sokolowski — Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstraße 12, 53115 Bonn, Germany

Heteroepitaxy of insulators and ionic materials is of basic interest for understanding the interactions at the respective interfaces. So far the heteroepitaxy of alkalihalides has been studied by various groups using single crystals and RHEED [1,2]. In the present work, we studied the epitaxy of NaCl on KCl by SPA-LEED. In order to avoid charging effects in the electron diffraction, we used thin films of KCl(100) epitaxially grown on a Ag(100) surface. For different growth temperatures we observed two different growth modes: At 300 K, we get highly disordered, but closed layers of NaCl. We observe a coherent transition between the lattices of KCl and NaCl and a relaxation of the NaCl lattice constant after few monolayers. At 500 K, we observe the formation of ordered NaCl islands with uncovered areas of the KCl and Ag surfaces in between. The quality of the NaCl films can also be characterized by optical spectra of isolated PTCDA molecules deposited on these. On NaCl structures grown at 500 K, the spectra are broadened, which we explain by a large diversity of adsorption sites related to structural defects of the NaCl films. Supported by SFB 624.

[1] M. H. Yang, C. P. Flynn, Phys.Rev.Lett 62 (1989) 2476.

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O 35.64 Tue 18:15 Poster B1

Investigation of the surface morphology of ultrathin hex-Pr_2O_3 on Si(111) — •Jari Rodewald[1], Henrik Wilkens[1], Sebastian Gevers[1], Marvin Zoellner[2], Thomas Schroeder[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49069 Osnabrück — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

The surface morphology and chemical composition of hex-Pr_2O_3 grown by molecular beam epitaxy (MBE) on Si(111) is studied by Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED) and Auger Electron Spectroscopy (AES), respectively.

The samples were capped with an amorphous germanium layer, since hex-Pr_2O_3 is instable under ambient conditions. In a first step the removal of the capping layer is investigated. Perfect thermal removal was achieved for annealing at 500°C sample temperature in 10^{-6}mbar oxygen atmosphere. X-Ray Diffraction (XRD) reveals that the hexagonal structure of the entire praseodymia film is preserved during the removal process.

The Spot profile analysis resulted in a surface model consisting of single atomic step heights of the complete hex-Pr_2O_3 unit cell. Also, the grain size and terrace width are determined.

O 35.65 Tue 18:15 Poster B1

CoO(111) bilayer on Ir(100) revisited: An incommensurate Moiré overlayer with strong local binding — Florian Mittendorfer[1], •Josef Redinger[1], Raimund Podloucky[2], Michael Weinert[3], Carsten Tröppner[4], Tobias Schmitt[4], Martina Reuschl[4], Lutz Hammer[4], and M. Alexander Schneider[4] — [1]Applied Physics, TU Vienna, Austria — [2]Physical Chemistry, Vienna University, Austria — [3]Dept. of Physics, University of Wisconsin-Milwaukee, USA — [4]Solid State Physics, University Erlangen-Nuremberg, Germany

Although a CoO(111) bilayer on Ir(100) is a relaxed overlayer with a very strong structural response to the lateral modulation of the interface [1], it turns out to form an one-dimensional incommensurate Moiré structure [2] as revealed by large-scale, low-temperature STM topographies. Despite the non-commensurability of the film, the binding to the substrate is site specific, where the strong lateral modulation of the structural elements within the oxide film can be understood as a combination of the lateral variation in the Co-Ir binding potential and additional O-Ir binding. This is in agreement with recent DFT investigations of the complex magnetism in a CoO(111) bilayer on Ir(100) [3], which found energetic degeneracies with respect to registry shifts of the CoO(111) film along the [011] direction and predicted a registry shifted structure to be equally stable as the LEED structure in [1].

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O 35.66 Tue 18:15 Poster B1

Surface structure of crystalline Ce_7O_{12} films on Si(111) studied by LEED and XPS — •Olga Schuckmann[1], Henrik Wilkens[1], Robert Oelke[1], Marvin H. Zoellner[2], Andreas Schaefer[3], Thomas Schroeder[2], Marcus Bäumer[3], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]IHP Frankfurt (Oder), Germany — [3]Institute for Applied and Physical Chemistry, University of Bremen, Germany

Cerium oxide is a particularly interesting material for various applications in the field of catalysis due to its high oxygen mobility and storage capability. Hence, the knowledge of the surface structure and oxygen vacancy formation is necessary to understand the elementary catalytic processes as well as the ionic conductivity.

Stoichiometric and structural changes induced by reducing epitaxial cub-$CeO_2(111)$ films grown on Si(111) was studied using low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS). The composition was determined by means of factor analysis of the Ce 3d X-ray photoemission spectra. The results indicate that Ce^{4+} cations are reduced to Ce^{3+} by heating the cerium dioxide films in ultrahigh vacuum. At an annealing temperature of 1070 K a transition from a (1x1) CeO_2 surface to a $(\sqrt{7}x\sqrt{7})R19.1^\circ$ superstructure takes place. The analysis of the XP spectra reveals a ratio of 57% of Ce^{3+} and thus a stoichiometry of Ce_7O_{12} for the reconstructed surface.

O 35.67 Tue 18:15 Poster B1

Surface investigation of ceria films on Si(111) after post deposition annealing

— •Robert Oelke[1], Henrik Wilkens[1], Olga Schuckmann[1], Reinhard Olbrich[1], Marvin H. Zoellner[2], Thomas Schroeder[2], Michael Reichling[1], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

The surface morphology of 250 nm crystalline $CeO_2(111)$ films grown on hex-Pr_2O_3/Si(111) annealed under UHV conditions was investigated with spot profile analysis low energy electron diffraction (SPA-LEED) and atomic force microscopy (AFM).

The two dimensional LEED pattern of the untreated sample exhibits triangular shaped reflexes due to surface facets, which is also confirmed by AFM measurements. Furthermore, the terrace width and single atomic step height are determined by an energy dependent analysis of the central diffraction spot profile.

Above an annealing temperature of 930 K the shape of the diffraction spots changes indicating that the surface facets vanish, which is also observed in the AFM images. Moreover, the AFM results show very large terraces.

Furthermore, several superstructures are observed at elevated temperatures indicating a periodic order of oxygen vacancies during reduction.

O 35.68 Tue 18:15 Poster B1

Oxidation of graphene on Rh(111)

— •Karin Gotterbarm, Wei Zhao, Oliver Höfert, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91052 Erlangen

We studied the oxidation of graphene sheets grown on a Rh(111) single crystal surface. The graphene was grown by chemical vapor deposition of propylene at 920 K. The growth process and oxidation were studied in-situ by fast XPS performed at the synchrotron facility BESSY II. The lattice mismatch of graphene on the Rh(111) surface induces corrugation of the graphene sheet leading to two separated signals in the C 1s region[1]. These two signals become most pronounced for graphene layers with a low defect density. The oxidation of graphene was investigated depending on oxygen pressure, temperature and graphene layer quality. We found sigmoidal reaction kinetics indicating the following reaction mechanism: The oxidation starts at defect sites, inducing an induction period. With more free adsorption sites the reaction rate increases until most of the graphene is oxidised. The remaining carbon decays exponentially according to pseudo first order kinetics. The influence of the quality of the graphene layer on the reaction rate supports the assumption that oxidation starts at the defect sites.

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O 35.69 Tue 18:15 Poster B1

Can graphene be turned into a topological insulator?

— •Carola Strasser[1], Bart Ludbrook[2], Andrea Damascelli[2], Christian R. Ast[1], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Quantum Matter Institute, UBC, Vancouver, BC V6T 1Z4, Canada — [3]Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

In 2005 Kane and Mele [1] claimed that graphene opens a band gap at very low temperatures due to spin orbit coupling (SOC) and becomes a quantum spin Hall insulator. Since the SOC is very weak in carbon atoms the size of the gap is very small and experimentally not observable. Recently Weeks et al. [2] showed theoretically that the intrinsic SOC can be enhanced by depositing small amounts of heavy adatoms on top of a graphene sheet. The electrons which hop on the adatoms and back to the graphene sheet induce higher SOC. Calculations showed that this gives rise to a band gap of Δ_{SOC}=25 meV at the K-point which should be observable with spectroscopic methods.

We performed angular resolved photoemission spectroscopy measurements at very low temperatures on epitaxial graphene on SiC. To induce higher SOC we decorated the sample with small amounts of Thallium. We observed small doping effects due to electron transfer from the adatoms to the graphene sheet. The doping level is increasing with coverage until it saturates. The band shift and indications for a gap opening will be presented in detail.

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O 35.70 Tue 18:15 Poster B1

High Temperature Angle-Resolved Photoemission from Graphene

— Søren Ulstrup[1], •Marco Bianchi[1], Richard C. Hatch[1], Dandan Guan[1], Alessandro Baraldi[2,3], Dario Alfé[4], and Philip Hofmann[1] — [1]Dep. of Physics and Astronomy, iNano Centre, Aarhus University, Denmark — [2]Dep. of Physics and CENMAT, University of Trieste, Italy — [3]Lab. TASC INFM-CNR, AREA Science Park, Trieste, Italy — [4]Dep. of Physics and Astronomy, TYC@UCL, University College London, United Kingdom

The temperature-dependent electronic structure and electron-phonon coupling of weakly doped supported graphene is studied by angle-resolved photoemission spectroscopy at temperatures up to 1300 K. The finding of an extremely weak electron-phonon coupling is accompanied by the observation of a complex and dramatic change in the graphene carrier density and type. Ab-initio molecular dynamics simulations show that these changes can be related to the temperature-dependent dynamic interaction with the Ir(111) substrate and are mainly caused by fluctuations in the graphene-substrate distance.

O 35.71 Tue 18:15 Poster B1

Defect creation in graphene by swift heavy ion irradiation

— •Alexander Levish, Oliver Ochedowski, Hanna Bukowska, and Marika Schleberger — Universität Duisburg-Essen, Duisburg, Germany

Graphene, a single layer of carbon atoms arranged in a honeycomb lattice, is envisaged to play an important role in several future applications like semiconductor devices, solar cells, biosensors, fuel cells, etc. The irradiation of graphene with different kind of ions is still a new and promising way to alter the physical properties of graphene. In case of swift heavy ions (SHI) with kinetic energies in the MeV regime it has already been shown that SHI can be used to create closed bilayer edge structures on exfoliated single layer graphene sheets on a wide variety of substrates. Here, using Raman spectroscopy we will show that SHI can be used to create defects even in suspended graphene sheets. Moreover, atomic force microscopy is applied to study the formation of closed bilayer edge structures upon SHI irradiation. We demonstrate that this process is influenced by the crystalline quality of graphene as well as the orientation of the graphene lattice with respect to the ion trajectory.

O 35.72 Tue 18:15 Poster B1

Characterization of graphene on ferromagnetic materials

— •Torsten Veltum, Hendrik Bettermann, and Mathias Getzlaff — Heinrich-Heine-Universität Düsseldorf

In the past few years graphene has gained the attention of scientists due to its unique mechanical and electrical properties. Perfect spin filtering has been predicted for interfaces between graphene and ferromagnetic materials. Iron nanoparticles have been shown to exhibit an in-plane magnetization alligned to that of a supporting thin film of a ferromagnetic material. In this study we want to discuss the properties of ferromagnetic surfaces regarding their suitability for graphene synthesis and their interaction with ferromagnetic nanoparticles.

Thin films of ferromagnetic materials like Ni, Co or Fe are prepared by electron beam evaporation on a W(110) crystal under ultra-high vacuum conditions. To achieve a structurally ordered monolayer graphene on the ferromagnetic substrate we use chemical vapor deposition with propylene. The structure of the thin film system is characterized insitu by means of scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and Auger electron spectroscopy (AES).

The well-characterized Fe nanoparticles are produced by a continuously working arc cluster ion source (ACIS), mass-selected by an electrostatic quadrupole ($\Delta m/m = 10\%$) and subsequently deposited on the single-layer graphene under softlanding conditions. The structural analysis of the nanoparticles is carried out by STM.

O 35.73 Tue 18:15 Poster B1

Hydrogenation of Graphene and Boron-doped Graphene — •Wei Zhao, Karin Gotterbarm, Olive Höfert, Christoph Gleichweit, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

We studied the hydrogenation and dehydrogenation of pristine graphene and boron-doped graphene prepared on a Ni(111) surface. We used in-situ temperature programmed high-resolution XPS to study the degree of hydrogenation and the thermal stability of the resulting layer. B-doped graphene layers with differing boron contents of 0-5% were hydrogenated at 170 K by atomic hydrogen. Additionally we also studied graphene layers intercalated with gold and still found hydrogenation. Hydrogenation at elevated exposures led to etching of the graphene layer by the atomic hydrogen. This process is hampered by boron doping. After gold intercalation we found that the etching is suppressed.

O 35.74 Tue 18:15 Poster B1

Coulomb- and phonon-induced inter-Landau-level carrier dynamics of graphene in a magnetic field — •Florian Wendler, Andreas Knorr, and Ermin Malić — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Motivated by a recent experiment [1], we investigate the relaxation dynamics of Dirac electrons in graphene in the presence of a magnetic field. In the experiment, a pump-probe setup is used to measure the relaxation times of electrons in the energetically lowest Landau levels. Exploiting the optical selection rules emerging in a magnetic field as well as the graphene-specific non-equidistant Landau-level splitting, single Landau-level transitions can be selectively measured using circularly polarized light. Here, we apply a theoretical approach within the framework of the density matrix formalism [2], which allows us to microscopically track the equilibration of excited electrons in reciprocal space. We investigate the impact of Coulomb- and phonon-induced relaxation channels between the lowest Landau levels. We find a phonon-dominated picosecond decay time confirming the experimentally observed trend. Furthermore, we discuss the importance of disorder-assisted carrier-phonon scattering processes, which are known to be important for the relaxation dynamics close to the Dirac point [3].

[1] M. Mittendorf, S. Winnerl, and M. Helm (unpublished)
[2] E. Malić et al., Phys. Rev. B 84, 205406 (2011)
[3] J.C.W. Song et al., Phys. Rev. Lett. 109, 106602 (2012)

O 35.75 Tue 18:15 Poster B1

Excitonic oscillator strength of metallic and semiconducting carbon nanotubes — •Eike Verdenhalven and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

The intrinsic oscillator strength of single-walled carbon nanotubes (CNTs) plays a crucial role for the optical assignment and the estimation of the abundance of a given nanotube species in a sample. In particular, pronounced absorption intensities do not necessarily correspond to a high abundance in the investigated sample. Based on a microscopic approach, we calculate excitonic absorption spectra for a variety of semiconducting and metallic CNTs allowing us to investigate the diameter and the chirality dependence of the oscillator strength for individual carbon nanotubes [1,2]. Our calculations reveal a pronounced chiral dependence, which strongly varies for different optical transitions and nanotube families. We find that semiconducting CNTs with large chiral angles (armchair-like) and large diameters show the most pronounced absorption intensities confirming the experimentally observed trend [3].

[1] Eike Verdenhalven and Ermin Malic, "Excitonic oscillator strength of metallic and semiconducting carbon nanotubes", submitted for publication (2012)

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O 35.76 Tue 18:15 Poster B1

Work function study and surface photovoltage phenomena of graphene on SiC — •Samir Mammadov[1], Jürgen Ristein[1], and Thomas Seyller[1,2] — [1]Lehrstuhl für Technische Physik Erwin-Rommel-Str. 1 91058 Erlangen — [2]Technische Universität Chemnitz Institut für Physik * Technische Physik Reichenhainer Straße 70 09126 Chemnitz

Subject of this study is the investigation of the work function and bandbending of epitaxial graphene(EG) on SiC. Two types of samples were investigated: regular EG *lms and H-intercalated EG *lms, referred to as quasi-freestanding graphene (QFG). EG *lms were formed by thermal decomposition on the Si-face of 6H-SiC substrates and QFG samples were formed by subsequentially intercalating EG samples by hydrogen. The work function and it*s dependance on the number of graphene layers was precisely determined for each type of sample by the Kelvin method. Additionally, laser induced surface photovoltage was measured in situ. The results are used to construct a full band diagram for the graphene/SiC heterostructure.

O 35.77 Tue 18:15 Poster B1

Band renormalization, mini-cones and Fermi surface discontinuities in epitaxial graphene on SiC(0001) by Cu intercalation — •Stiven Forti[1], Konstantin V. Emtsev[1], Alexei A. Zakharov[2], Camilla Coletti[3], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]MAX Lab, Lund University, Box 118, Lund, 22100, Sweden — [3]Center for Nanotechnology Innovation @ NEST, Istituto Italiano di Tecnologia, Piazza San Silvestro 12, 56127 Pisa, Italy

The interaction of graphene with transition metals as well as the effects of a periodic perturbation on the graphene's band structure are fields of great interest. In this work we present photoemission spectroscopy (PES), low-energy electron diffraction (LEED) and microscopy (LEEM) to study the effects of an ordered layer of Cu atoms intercalated under epitaxial graphene (EG) on SiC(0001). By means of angle-resolved photoelectron spectroscopy (ARPES) measurements, we observed that the intercalated graphene is effectively decoupled from the substrate and the interfacial Cu layer imposes both a strong n-doping and a periodic potential, which deeply affect the graphene's band structure. The site-specific interaction between Cu and graphene, together with the chiral nature of the graphene's carriers, produce the development of minicones (mCs) located along the boundaries of the graphene's Brillouin zone. Mini band-gaps are observed at the mCs vertexes and the Fermi surface exhibits discontinuities caused by the emergence of new electronic states associated with the mCs.

O 35.78 Tue 18:15 Poster B1

Synthesis of epitaxial graphene on C-face SiC: influence of growth conditions — •Timo Schumann[1], Inna Shteinbuk[1,2], Myriano H. Oliveira Jr.[1], J. Marcelo J. Lopes[1], and Henning Riechert[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]City College of New York, New York, United States

Surface Si depletion of hexagonal SiC offers the possibility of producing high-quality graphene directly on an insulating substrate. However, while on the Si-face monolayer graphene can be prepared on a large area, on the C-face a precise control over the number of layers is hard to be achieved. Nevertheless, even films with many carbon layers behave like decoupled monolayer graphene sheets on C-face SiC, potentially offering higher electron mobilities than graphene layers on Si-face SiC. We investigated the influence of the growth conditions, *i.e.* temperature, growth time and environment (Argon, vacuum, enclosed space) on the growth of epitaxial graphene on C-face SiC. The quality of the resulting layers is investigated by means of atomic force microscopy, Raman spectroscopy and magnetotransport measurements. This work aims to offer a guideline for reproducible production of uniform and high-quality graphene sheets.

O 35.79 Tue 18:15 Poster B1

Optical properties of bilayer graphene — •Faris Kadi and Ermin Malić — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

We present a microscopic study of the optical properties of Bernal-stacked bilayer graphene. In particular, we show the excitonic absorption and conductance for all possible optical transitions. Our theoretical approach is based on the density matrix formalism in combination with tight-binding wave functions [1]. In contrast to the linear band structure of monolayer graphene, bilayered graphene exhibits four parabolic bands near the Dirac point. This results in bilayer-characteristic features in the absorption spectrum. We find that the low energy spectrum exhibits a pronounced peak, which is induced by interlayer transitions around the Dirac point. In the ultraviolet region, the spectrum exhibits two energetically close absorption peaks resulting from interband transitions at the saddle point of the Brillouin zone. We discuss the optical matrix element determining the strength of different optical transitions as well as the Coulomb interaction accounting for energy renormalization and formation of strongly bound electron-hole pairs.

[1] E. Malić, T. Winzer, E. Bobkin, and A. Knorr, Phys. Rev. B 84, 205406, (2011)

O 35.80 Tue 18:15 Poster B1

Atomistic simulations of defects in bilayer graphene — •Konstantin Weber and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

Simple Lennard-Jones-based Van-der-Waals potentials are not capable to describe simultaneously the correct depth and corrugation of the interaction potential between two graphene sheets since they are too smooth and do not capture the short-ranged orbital overlap between graphene pi-electron systems. To cure this problem, Kolmogorov and Crespi [1] proposed a registry-dependent interlayer potential which we implemented into the LAMMPS software package in combination with the classical interatomic AIREBO potential [2] for the covalent carbon–carbon bonds. The improvements in the description of bilayer graphene with this new potential will be discussed and first results on the structure and energy of dislocations in bilayer graphene will be shown.

[1] A. Kolmogorov, V. Crespi, *Phys. Rev. B* **71**, 235415 (2005).

[2] D.W. Brenner, et al., *J. Phys.: Condens. Matter* **14**, 783 (2002).

O 35.81 Tue 18:15 Poster B1

Torque magnetometry on large-area graphene — •Matthias Block[1], Stephan Albert[1], Stefanos Chalkidis[1], Florian Speck[2], Felix Fromm[2], Thomas Seyller[3], Marc Wilde[1], and Dirk Grundler[1] — [1]Technische Universität München, Department Physik E10, James-Franck-Str. 1, 85747 Garching b. München — [2]Universität Erlangen, Lehrstuhl für Technische Physik, Erwin-Rommel-Str. 1, 91058 Erlangen — [3]Technische Universität Chemnitz, Institut für Physik, Technische Physik, Reichenhainer Str. 70, 09126 Chemnitz

Torque magnetometry performed at helium temperatures allows one to gain insight into the electronic properties of two-dimensional electron systems. Graphene with its unique electronic properties is in particular interesting. While much of fundamental knowledge about graphene was learned from small-sized exfoliated graphene, it is important for our technique to study large areas of graphene. We use graphene epitaxially grown on SiC as it offers similarly high electronic quality and is provided in wafer-scale sizes. For our experiment we use micromechanical cantilevers which are designed for sample sizes of 1.2 mm × 2 mm. We use SiC-graphene which has been characterized by Raman spectroscopy and atomic force microscopy to determine the amount of monolayer graphene. We report on our results of the magnetization measurements based on torque magnetometry. We acknowledge financial support by the DFG via project WI3320/1-1 in SPP 1459.

O 35.82 Tue 18:15 Poster B1

Downsizing graphene: routes towards epitaxial graphene nanoribbons (EGNR) on SiC — •Alexander Stöhr, Stiven Forti, and Ulrich Starke — Max Planck Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

In recent years, great efforts have been spent in trying to realize a facile and scalable technique to produce graphene-based nanostructures for logic electronics. In this work we illustrate different experimental approaches to achieve quasi-1D structures based on epitaxial graphene (EG) on SiC. We present our first results about vicinal 4H-SiC surfaces, the 6H-SiC$(1\bar{1}09)$ facet and anisotropic etching of graphene by means of metallic nanoparticles. Vicinal SiC surfaces offer a promising template for producing 1D graphene nanostructures on a wafer size due to the self-ordering of narrow terraces. Narrow trenches can be patterned into graphene by self-organized catalytic etching with metallic nanoparticles. By combination with H-intercalation of the buffer layer free-standing structured monolayer graphene can be obtained. We show nanoparticles deposition in a monodispersed distribution and the catalytic propagation in preferential directions. The bottom-up approach for definition of graphene nanostructures is of crucial importance since it avoids possible contaminations typical of the ex-situ lithographical approach. Nevertheless, patterned graphene relaxes into basal plane terraces and facets (e.g. $(1\bar{1}09)$) when annealed at elevated temperatures. To understand the graphene growth mechanism on those facets we investigated the $(1\bar{1}09)$-surface of 6H-SiC itself.

O 35.83 Tue 18:15 Poster B1

Transfer of Ni grown graphene onto an insulating YSZ substrate — •Samuel Grandthyll[1], Stefan Gsell[2], Michael Weinl[2], Matthias Schreck[2], Stefan Hüfner[1], Frank Müller[1], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, 66041 Saarbrücken, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Graphene has been grown epitaxially on several Ni(111)/YSZ/Si(111) multilayer samples by chemical vapor deposition (CVD) of the precursor acetone [1]. The aim was to use the nickel film (thickness approximately 150 nm) as a catalyst for precursor fragmentation and graphene growth. Once the graphene film has formed, the thin metal film can be removed by etching in order to transfer graphene onto the underlying YSZ (Yttria-Stabilized Zirconium oxide) insulator.

During this synthesis route the samples were characterized in each step by several techniques, such as X-ray Photoelectron Spectroscopy (XPS), X-ray Photoelectron Diffraction (XPD), Low Energy Electron Diffraction (LEED), and Fermi Surface Mapping (FSM) by Angular Resolved Ultraviolet Photoelectron Spectroscopy. The results reveal that the transfer of ordered graphene layers is possible by this preparation mechanism.

References:

[1] J. Phys.: Condens. Matter 24 (2012) 314204

O 35.84 Tue 18:15 Poster B1

Electronic states of spatially coordinated graphene nanoribbons on Ag(775) — •Alexander Timmer[1], Nabi Aghdassi[1], Dingyong Zhong[1], Xinliang Feng[2], Klaus Müllen[2], Harry Mönig[1], Lifeng Chi[1], Helmut Zacharias[1], and Harald Fuchs[1] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

On-surface covalent coupling of specific organic primer molecules on vicinal metal surfaces under UHV conditions represents a reliable technique to prepare well-arranged molecular surface patterns [1]. Based on our previous work on Au(788) we created an array of precisely-aligned armchair graphene nanoribbons on Ag(775) [2]. The electronic properties of these GNRs are analyzed with angle-resolved ultraviolet photoemission spectroscopy (ARPES), angle-resolved inverse photoemission (KRIPES), and scanning tunneling microscopy (STM), which allows for the determination of the 7-aGNRs bandgap. This study is particularly focusing on the role of the metal-substrate interaction and possible doping effects [3]. The data for 7aGNRs on Ag(775) are compared to LDA and GW calculations conducted for isolated aGNRs and to a semiclassical model incorporating substrate polarization effects as well as to our previous study of 7aGNRs on Au(788) [4]. The results indicate that the chosen substrate plays a significant role for the electronic properties of the considered systems. [1] J. Cai et al., Nature 466, 470 , [2] S. Linden et al., PRL 108, 216801 , [3] D. Prezzi et al., Phys. Rev B 84, 041401(R) , [4] L. Liang et al., Phys. Rev B 86, 195404

O 35.85 Tue 18:15 Poster B1

Graphene growth by Faco-to-Face method and occurrence of step bunching process — •Philipp Ansorg, Thomas Druga, Martin Wenderoth, and Rainer G. Ulbrich — Institute of semiconductor physics, Göttingen, Germany

Studying the outstanding properties of graphene requires a reliable production process. We have grown epitaxial graphene on n-doped 6H-SiC(0001) under UHV conditions and determined the influence of temperature on graphene growth. In addition an experimental arrangement after Yu et al. [1], called *Face-to-Face* method, was used for the preparation of graphene. The quality of the sample surface was studied by Atomic Force Microscopy under ambient conditions. Domains of graphene up to $3 \times 30 \mu m^2$ are found. Besides determining optimal conditions for graphene growth we observed the mechanism of *step bunching.* The height of the final steps is equivalent to multiples of three times the height of a SiC-bilayer, pointing to a step bunching process of higher order. The width of the graphene domains corresponds to multiples of three times the width of substrate terraces first discovered by Hupalo et al. [2].

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Spectroscopy and Related Phenomena **184** (2011), p. 100

O 35.86 Tue 18:15 Poster B1

Epitaxial growth of graphene on copper foil — •Christian Raidel[1], Felix Fromm[1], Roland Koch[1], Johannes Jobst[2], and Thomas Seyller[1,3] — [1]FAU Erlangen-Nürnberg, Technische Physik, Erlangen, Deutschland — [2]FAU Erlangen-Nürnberg, Angewandte Physik, Erlangen, Deutschland — [3]TU Chemnitz, Institut für Physik, Chemnitz, Deutschland

We investigated the growth of epitaxial graphene on commercial copper foil by atmospheric pressure chemical vapor deposition using methane and pyridine as precursors. Pyridine was used to incorporate nitrogen as a dopant into graphene. For optimal growth conditions the copper foils were pretreated by electro-polishing and annealed at elevated temperatures for achieving low defect densities and large grains. The growth of the graphene layers was studied by x-ray photoelectron spectroscopy (XPS), while scanning electron microscopy (SEM) was used to determine structural details of the layers. In addition, Raman spectroscopy was employed to investigate the quality of the layers.

XPS measurements of the as-grown films revealed that the growth resulted in multi-layer graphene. Transfer of the graphene layers from the cupper foil onto SiO_2 wafers was also studied. The XPS spectra remained basically unchanged. On the other hand, Raman spectroscopy indicates an increase in strain and defects after the transfer. Graphene layers grown with pyridine were transferred using a nitrogenfee resist. In that case, XPS showed the existence of nitrogen in the layer. The origin of the nitrogen content, however, cannot be absolutely pinpointed to the employed precursor, as will be discussed in the presentation.

O 35.87 Tue 18:15 Poster B1

Organic molecular self-assembly on epitaxial graphene — •Alexei Nefedov[1], Wenhua Zhang[2], Michael Naboka[1], Hikmet Sezen[1], Liang Cao[2], and Christof Woell[1] — [1]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Leopoldshafen, Germany — [2]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, PRC

The adsorption of organic molecules as pentacene (Pn) and terephthalic acid (TPA) on a single layer of graphene grown epitaxially on Ni(111) has been investigated by means of near-edge X-ray absorption fine structure (NEXAFS) spectroscopy and X-ray photoelectron spectroscopy (XPS) at room temperature. The assignment of the NEXAFS-resonances was aided by ab-initio calculations by StoBe package. For coverages up to a monolayer the molecular plane of TPA adopts a parallel orientation with regard to the epitaxial graphene (EG) layer. Deprotonantion of TPA molecules at one monolayer coverage can be excluded. For TPA multilayers, the molecular plane is tilted on average by approximately 45° with respect to the sample surface. Pentacene molecules demonstrate a dependence of their orientation and electronic structure on the coverage. The observed effects will be discuss in detail during presentation.

O 35.88 Tue 18:15 Poster B1

Investigation of graphene contact resistivity on semi-insulating silicon carbide by Kelvin Probe Force Microscopy — •Felix Lüpke, Martin Wenderoth, Thomas Druga, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany

We present first Kelvin Probe Force Microscopy (KPFM) and simulation of the lateral charge transport across few-layer graphene on the semi-insulating 6H-SiC(0001) surface. After preparation of the SiC crystal using common methods [1], atomically flat graphene layers of up to few hundred nm in lateral dimension were observed. Gold electrodes were prepared on top of the graphene layer by thermal evaporation through a shadow mask. For transport measurements a lateral voltage was applied across the sample at the gold electrodes in addition to the usual alternating tip-sample voltage used for KPFM [2]. The potential measured by KPFM is an overlay of the local work function of the sample and the voltage drop across the graphene layer. By subtracting measurements of reverse lateral bias the voltage drop was extracted. We find an ohmic behavior of the contacted graphene layer and a graphene sheet resistance of 1 kΩ/sq. By comparing the experimental transport measurements with a resistance network simulation the contact resistivity between graphene and a gold electrode can be determined to $< 1 \times 10^{-5}$ Ω/cm^2.

[1] Forbeaux, I.; Themlin, J.-M.; Debever, J.-M. Phys. Rev. B, 1998, 58, 24 [2] Yan, L.; Punckt, C.; Aksay, I. A.; Mertin, W.; Bacher, G. Nano Lett., 2011, 11

O 35.89 Tue 18:15 Poster B1

Two-photon photoemission studies of graphene on Ir(111) — •D. Nobis[1], D. Niesner[1], Th. Fauster[1], M. Kralj[2], M. Petrović[2], P. C. Yeh[3], S. Y. Hong[3], W. Jin[3], J. Dadap[3], and R. M. Osgood[3] — [1]Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Institut za fiziku, Bijenička 46, HR-10000 Zagreb, Croatia — [3]Columbia University, New York, NY 10027, USA

Graphene can be grown on Ir(111) with high quality by decomposition of hydrocarbons [1]. The band structure of this system has been studied with various techniques [2,3]. We have used two-photon photoemission (2PPE) to study the image-potential states of graphene on Ir(111). Using monochromatic 2PPE (photon energies $3.99 - 4.86$ eV) and bichromatic 2PPE (pump pulse 4.77 eV, probe pulse 1.59 eV) we observe two $n = 1$ image-potential bands. The main peak agrees with previous data [3]. The weaker second band has a slightly larger binding energy and effective mass.

We discuss possible origins of the second band: (a) Splitting in odd and even bands with respect to the graphene layer [4]. (b) Umklapp bands or (c) localized states due to the moiré structure of graphene on Ir(111) [5].

[1] van Gastel, R. *et al.*, Appl. Phys. Lett. **95** (2009) 121901
[2] Kralj, M. *et al.* Phys. Rev. B **84** (2011) 075427
[3] Niesner, D. *et al.*, Phys. Rev. B **85** (2012) 081402(R)
[4] Bose, S. *et al.*, New J. of Physics **12** (2010) 023028
[5] Armbrust, N. *et al.*, Phys. Rev. Lett. **108** (2012) 056801

O 35.90 Tue 18:15 Poster B1

Magnetism in graphene induced by the adsorption of atmospheric species — •Nora Jenny Vollmers[1], Eva Rauls[1], Wolf Gero Schmidt[1], Uwe Gerstmann[1], and Francesco Mauri[2] — [1]Festkörpertheorie, Department für Naturwissenschaften, Universität Paderborn, Paderborn, Germany — [2]Institut de Minéralogie et de Physique des Milieux Condensés, Université Pierre et Marie Curie, Paris, France

Besides its outstanding properties with respect to conductivity the two-dimensional material graphene has attracted a still increasing deal of interest due to an unconventional magnetism. Although, ideal graphene is nonmagnetic, already the presence of non-metallic defects induces magnetism in the material. Graphene has, thus, attracted great interest as a metal-free magnetic meterial. The defects can be either introduced intentionally by irradiation or doping, however, in most cases they are unavoidable by-products of material growth, or simply by the exposure to air.

We use density functional theory and the Quantum Espresso package to investigate the influence of atmospheric species on monolayer graphene. Our main focus lies on the question, how the different atoms influence the electronic and magnetic properties of the substrate. We study the adsorbtion and substitutional incorporation of hydrogen, oxygen and nitrogen by analyzing the calculated total energies, magnetic moments and simulated spin-polarized STM images.

O 35.91 Tue 18:15 Poster B1

N-doped single-layer graphene by conversion of aromatic self-assembled monolayers — •Oliver Reimer[1], Nils-Eike Weber[1], Stefan Wundrack[2], Rainer Stosch[2], and Andrey Turchanin[1] — [1]Faculty of Physics, University of Bielefeld, 33615 Bielefeld, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

N-doped graphene sheets are promising for applications in transparent conductive coatings, supercapacitors or as catalysts for oxygen reduction. However, controllable fabrication of this material is not yet well established. Here, we present a molecular route to N-doped single-layer graphene based on electron-beam-induced crosslinking of N-containing aromatic self-assembled monolayers on copper foils and their subsequent temperature-induced conversion into graphene. We characterize this conversion as well as structural and chemical properties of the formed graphene sheets by complementary surface science techniques (X-ray photoelectron microscopy, low energy electron diffraction) and Raman spectroscopy. Functional properties of the formed single-layer graphene are tested by electrical measurements on oxidized silicon wafers.

O 36: Poster Session II (Organic films and electronics, photoorganics; Nanostructures; Plasmonics and nanooptics, Surface chemical reactions and heterogeneous catalysis, Surface dynamics)

Time: Tuesday 18:15–21:45 Location: Poster B2

O 36.1 Tue 18:15 Poster B2

Molecular Junctions Using Epitaxial Monolayer Graphene Electrodes — •Konrad Ullmann, Daniel Waldmann, Stefan Ballmann, and Heiko Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Germany

We report on a method to fabricate epitaxial monolayer graphene electrodes with nanometer separation grown on silicon carbide. The nanometer-gap is formed by feedback controlled electroburning of carbon atoms in presence of oxygen. A gapsize of approximately 1nm is extracted from the tunneling current.

Using these gaps we are able to form molecular junctions. Subsequently I-V measurements of a molecule possessing fullerene anchor groups exhibit prominent peaks in differential conductance, which is typical for single-molecule junctions.

O 36.2 Tue 18:15 Poster B2

THz conductivity of graphene films derived from functionalized graphene dispersions — •Christoph Testud, Martin Fabritius, Rolf Mülhaupt, Hanspeter Helm, and Markus Walther — Freiburger Materialforschungszentrum (FMF), Freiburg, Deutschland

We report THz conductivity measurements on functionalized graphene films over the frequency range 0.1-1.5 THz. The films have been produced by depositing dispersions of single graphene sheets on a substrate. The conductivity is measured by THz TDS (time domain spectroscopy), which represents a contactless and non-destructive characterization technique. To check our results for consistency we compared our extrapolated dc-values with results from four-point probe measurements. Material parameters such as plasma frequency or charge carrier scattering rates are extracted from fits to our data using the Drude Smith model, which accounts for reduced conductivity due to charge carrier localization on the few micrometer sized graphene sheets.

O 36.3 Tue 18:15 Poster B2

A novel approach to the fabrication of ultrathin poly(ethylene glycol) films — Nikolaus Meyerbröker and •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

We present a novel approach to prepare stable, ultrathin poly(ethylene glycol) (PEG) films which can of potential interest for biotechnology and nanofabrication. The approach is based on cross-linking of multifunctionalized, star-branched PEGs (STAR-PEGs). A two component mixture of amine- and epoxy-terminated four-arm STAR-PEGs dissolved in chloroform was spin-coated on a flat substrate. The complementary STAR-PEGs were then cross-linked by gentle heating at 80°C, which was monitored in situ by infrared reflection-adsorption spectroscopy. The film thickness could be tuned in a controlled fashion from 4 to 200 nm as determined by ellipsometry. The films were biocompatible as could be expected for PEG-based materials. The films were stable in aqueous solutions but exhibited pronounced swelling behavior characteristic of hydrogels. Controlling the relative humidity, it was possible to adjust precisely the extent of swelling and perform it in controlled and reversible fashion. Further, immersing the films in solution of gold nanoparticles (AuNP) we succeeded to prepare PEG/AuNP composite films of variable density which exhibited interesting and potentially useful optical properties. Combining this procedure with standard lithographic techniques, AuNP patterns in the PEG-matrix were fabricated on a broad length scale.

O 36.4 Tue 18:15 Poster B2

The adsorption of silver on lignin and its precursors — •Sebastian Dahle[1,2], John Meuthen[1], Lienhard Wegewitz[1,3], Wolfgang Viöl[2], and Wolfgang Maus-Friedrichs[1,3] — [1]Institut für Energieforschung und physikalische Technologien, TU Clausthal — [2]Hochschule für angewandte Wissenschaft und Kunst — [3]Clausthaler Zentrum für Materialtechnik, TU Clausthal

The adsorption of silver on lignin is of great interest for the modification of wood surfaces with antibacterial coatings. The natural precursors during the biosynthesis of lignin are mainly the monolignols sinapyl alcohol and coniferyl alcohol. These have been used as model systems to get a better understanding of the interaction of silver with lignin. X-ray Photoelectron Spectroscopy, Ultraviolet Photoelectron Spectroscopy, Metastable Induced Electron Spectroscopy and Atomic Force Microscopy have been employed during the investigations, we observed a formation of silver nanoparticles upon the catalytic decomposition of the lignin as well as its precursors.

O 36.5 Tue 18:15 Poster B2

Coverage of $[\mathrm{Mn}_6^{\mathrm{III}}\mathrm{Cr}^{\mathrm{III}}]^{3+}$ SMMs on Surfaces Analyzed by Means of Kelvin Probe Force Microscopy — •Aaron Gryzia[1], Armin Brechling[1], Ulrich Heinzmann[1], Veronika Hoeke[2], and Thorsten Glaser[2] — [1]Molecular and Surface Physics, Bielefeld University — [2]Anorganic Chemistry I, Bielefeld University

$[\mathrm{Mn}_6^{\mathrm{III}}\mathrm{Cr}^{\mathrm{III}}]^{3+}$ is a Single-Molecule-Magnet and as such consists out of metal centers and organic compounds and ligands. These organic parts are one of the two main properties playing an important role regarding the adsorption of the molecule onto surfaces, such as e.g. mica and HOPG. The other one is the SMM's charge of 3+. The resulting dipole moment of the SMM layer influences the contact potential difference (CPD). By using FM-KPFM at UHV conditions we are able to determine the CPD of the sample. Furthermore the CPD depends on the interaction of the SMM with the substrate. By achieving molecular resolution inside the adsorbed layers we are able to determine aligning of SMMs in respect to the substrate. In addition we manipulate the adsorption sites in order to increase the order of the SMMs on the surface.

O 36.6 Tue 18:15 Poster B2

Electronic and adsorption properties of perylene-tetracarboxylic-dianhydride on Au(111) — •Stephan Stremlau[1] and Petra Tegeder[1,2] — [1]Freie Universität Berlin, Institut für Experimentalphysik — [2]Rubrecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut

Electronic and vibrational high resolution electron energy loss spectroscopy as well as temperature programmed desorption spectroscopy have been employed to gain insights into the adsorption behavior and the electronic properties of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Au(111). In the sub-monolayer regime the molecules adsorb in a planar geometry. With increasing coverage the molecules adopt a tilted configuration. Using sufficient high excitation energies of around 15.5 eV, the loss spectra in the multilayer regime show two strong electronic transitions at 2.3 and 2.5 eV. In the sub-monolayer regime only one transition at 2.6 eV is observed. The binding energy in the sub-monolayer range is 1.7(0.2) eV which is significantly lower than the recently published value of 2.5 eV [1].

[1] C. Wagner, N. Fournier, F.S. Tautz, R. Temirov, Phys. Rev. Lett., 109, 2012, 076102.

O 36.7 Tue 18:15 Poster B2

Impact of 2D structures on the back surface of solar cells on the absorption processes in these cells — •Jan Marc Stockschläder[1], Michael Jaax[2], Henning Fouckhardt[2], and Erich Runge[1] — [1]TU Ilmenau, 98693 Ilmenau, Germany — [2]TU Kaiserslautern, 67663 Kaiserslautern, Germany

Coupling light to the active medium of a solar cell is a crucial point for high efficiency. Therefore, structured substrates are studied to enhance the light matter coupling. Especially thin geometries are attractive because they have the potential to be fabricated low-cost. We present a 2D periodic structure based on the 1D double-periodic structures of Williamson et al. [1] as they already showed good surface-plasmon coupling capabilities. Furthermore, we analyse a structure based on Galois fields, which scatters incoming waves over a huge solid angle. This concept is well known for acoustic waves [2] and has recently been realized for the optical wavelength regime by M. Jaax et al. [3]. We show the yield enhancement as a substrate structure for solar cells.

[1] A. Williamson, E. McClean, D. Leipold, D. Zerulla, and E. Runge, *The design of efficient surface-plasmon-enhanced ultra-thin polymer-based solar cells* (APL **99**, 093307)

[2] T. J. Cox , P. D'Antonio, and Manfred Schroeder, *Acoustic Absorbers and Diffusers, Theory, design and application* (JASA **117**,3)

[3] M. Jaax, S. Wolf, B. Lägel, and H. Fouckhardt, *Optical reflective Galois scattering plates*, Presented at EOS Annual Meeting 2012, Aberdeen; (submitted to JEOS)

O 36.8 Tue 18:15 Poster B2

Tuning the work function of metal substrates by defined cleaning procedures and self assembling monolyers — •Marc Hänsel[1,3], Eric Mankel[1,3], Janusz Schinke[2,3], Wolfgang Kowalsky[2,3], Thomas Meyer[1,3], and Wolfram Jaegermann[1,3] — [1]Technische Universität Darmstadt, Materials Science Institute, Petersenstr. 32, Darmstadt — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik und Photonik, Schleinitzstr. 22, Braunschweig — [3]InnovationLab GmbH, Speyerer Str. 4, Heidelberg

Understanding the contact behavior of organic semiconductors is a prerequisite to improve the efficiency of devices. Self-assembling monolayers (SAMs) are an interesting and promising way to vary and to define the work function of substrate materials. To investigate the influence of the SAMs a reproducible substrate is required. For this 150nm thick gold layers were evaporated on flat silicon substrates. Different treatments (eg. oxygen and argon plasma only and in combination with an ethanol bath, heating under atmosphere and vacuum, UV radiation, argon sputtering) for cleaning were evaluated by photo emission spectroscopy (XPS/UPS). Depending on the procedure different levels of cleanness and work functions between 3.5eV and 5.3eV were achieved. The best reproducible and practical method was argon plasma treatment leading to work functions of 4.8eV and sub monolayer adsorbate concentrations. First experiments are done with selected SAMs like Perfluorodecanethiol. XPS measurements prove a Perfluorodecanethiol layer on the gold surface and Kelvin probe force microscopy shows a work function increase of 1eV compared to an untreated gold sample.

O 36.9 Tue 18:15 Poster B2

Charge carrier separation at P3HT-SiC based solar cells — •Andreas Lücke, André Konopka, Siegmund Greulich-Weber, Eva Rauls, Wolf Gero Schmidt, and Uwe Gerstmann — Universität Paderborn, Department Physik, Paderborn, Germany

Today the standard organic solar cells consist of a polymer-fullerene interface for charge carrier separation. In order to reduce the costs and to increase the separation effiency, substitutes for the fullerenes are highly desirable. Here, silicon carbide in its cubic polytype (3C-SiC) is a promising alternative, providing HOMO and LUMO positions similar to those of fullerenes [1]. Here we study numerically the geometry, electronic structure and electron transport properties of the P3HT-SiC interface. Thereby we use the Quantum Espresso Package [2] implementation of the density-functional theory. As a model for P3HT polymers interlocked P3HT chains are utilized.

In order to get a qualitative insight into the carrier separation process, the transition probability is calculated with a ballistic transport model. Particular emphasis is given onto the orientation of the P3HT molecules at the contact and the influence of van der Waals interactions.

[1] A. Konopka et al., Mat. Sci. Eng. 15, 012013 (2010).

[2] P. Giannozzi et al., J. Phys.:Condens. Matter 21, 395502 (2009); URL http://www.quantum-espresso.org

O 36.10 Tue 18:15 Poster B2

Structural and electronic properties of P3HT/SiC interfaces — •Andre Konopka, Siegmund Greulich-Weber, Andreas Lücke, Eva Rauls, Wolf Gero Schmidt, and Uwe Gerstmann — Universität Paderborn, Department Physik, Paderborn, Germany

Organic molecules have become an interesting new class of material in optoelectronic and photovoltaic applications. For organic photovoltaic applications a key issue is the separation of the photo-generated charges in the organic component. In organic molecules the charges are strongly bound and form excitons. In order to separate the electron and the hole a second material component has to be used. For many organic solar cell concepts fullerenes serve as an effective electron acceptor. It has been shown that inorganic semiconductors can also fill this role [1]. The necessary electronic structure for an effective transfer of the electrons into the acceptor material is closely related to states introduces to the system by the interface between the organic and inorganic components [2]. In this work we present different configurations of an organic-inorganic interface (P3HT/3C-SiC). Various binding situations of P3HT on the SiC surface have been calculated by density functional theory. We also studied the influence of van der Waals interaction on the structural and electrical properties of the interface. In comparison the situation for the typically used P3HT/PCBM material system are calculated.

[1] A. Konopka et al., IOP Conf. Series: Mat. Sci. Eng. 15, 012013 (2010). [2] A. Konopka et al., Mater. Res. Soc. Symp. Proc. Vol. 1322, (2011).

O 36.11 Tue 18:15 Poster B2

Simulation of charge transport in C_{60} self-assembled monolayers for applications in field-effect transistors — •Susanne Leitherer[1], Christof Jäger[2], Tim Clark[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, 91058 Erlangen, Germany — [2]Computer-Chemie-Centrum, Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstraße 25, 91052 Erlangen, Germany

Charge transport through self-assembled monolayers (SAMs), which are used in field-effect transistors [1], is studied employing the Landauer transport formalism. In particular, SAMs consisting of C_{60} as active layer, functionalized by octadecyl phosphonic acids and insulating alkyl phosphonic acids are investigated [1]. The structure of the SAMs is characterized by molecular dynamics simulations [2] and semi-empirical electronic structure calculations [3]. Using small test systems, we analyze pathways for efficient charge transport by examining the transmission eigenchannels [4]. Moreover, the dependence of the transport properties on the mixing ratio of the molecules is discussed.

[1] M. Novak *et al.*, Nano Lett. 11, 156 (2011)
[2] M. Novak *et al.*, Organic Electronics 11, 1479 (2010)
[3] C. Jäger *et al.*, Nat. Chem., submitted 2012
[4] J. C. Cuevas *et al.*, Phys. Rev. Lett. 80, 1066 (1998)

O 36.12 Tue 18:15 Poster B2

Photovoltaic effect of light carrying orbital angular momentum — •Jonas Wätzel, Andrey Moskalenko, and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale), Germany

Intensive research is devoted to the improvement of the efficiency of the photovoltaic elements by adjusting their material and structure properties. A promising alternative approach might be based on the adjustment of the structural properties of light before it is used to create currents in the cells, e.g. employing twisted light (TL) that is the idea followed in this presentation. TL is created routinely from usual light sources, e.g. via traversing a spiral wave plate that can be deposited onto the solar cell. One may think of enhancing the TL light intensity via self-focusing effect, an issue addressed recently. Strongly-focussed TL beams deliver additional opportunities to manipulate optical properties of nanostructures.

To explore the potential of TL for photovoltaics we investigate how the focussed TL beam influences an electron wave packet in a two-dimensional semiconductor stripe. We show that application of a TL beam results effectively in a voltage drop across the stripe with its sign being determined by the sign of the topological charge of TL. This is a photovoltaic effect that can be registered by measuring the generated voltage drop across the stripe and/or the current increase.

O 36.13 Tue 18:15 Poster B2

Deposition and spectroscopic study of Palladium complex on pyridine terminated quartz surface — •Deb Kumar Bhowmick[1,2], Helmut Zacharias[1,2], Wenchong Wang[1], and Lifeng Chi[1] — [1]Physikalisches Institut, WWU Münster, Münster, Germany — [2]Graduate School of Chemistry, WWU Münster, Münster, Germany

Particular interest exist in the formation of hybrid organic-inorganic material layers on semiconductor and insulator surfaces in which it is possible to control the function and properties by the nature and type of the incorporated metal ions [1]. A palladium (II) metal-organic complex with terpyridine ligand is synthesized in solution and deposited on a pyridine terminated quartz surface. The deposition process through organometallic complex can be one of the ways to functionalize surfaces with various organic molecules like dyes. This can be possible by further modifying the terpyridine ligand with different kind of organic molecules of interest. AFM, FT-IR spectroscopy and contact angle measurements are performed to characterize both the linker as well as organometallic functionalized quartz surfaces. The UV absorption spectrum yields two maxima at 353 nm and 370 nm of the organometallic functionalized quartz surface.

1] Altman, M.; Shukla, A. D.; Zubkov, T.; Evmenenko, G.; Dutta , P.; van der Boom, M. E. J. Am. Chem. Soc. 2006, 128, 7374-7382.

O 36.14 Tue 18:15 Poster B2

Glaser coupling at metal surfaces — •Hongying Gao[1], Hendrik Wagner[2], Dingyong Zhong[1], Armido Studer[2], and Harald Fuchs[1] — [1]Physikalisches Institut Muenster university,Wilhelm-Klemm-Straße 10, 48149 Münster — [2]Organisch-Chemisches Institut,Westfälische Wilhelms-Universität Münster,Corrensstraße 40, 48149 Münster

the Glaser coupling can be used highly efficiently to generate linear oligomer / polymer chains in spatial confinement at surfaces, which is impossible in conventional solution schemes. The generation of π-conjugated linear polymers directly at the interface is possible by using appropriate precursors and subsequent on-surface-coupling. It turned out that the Glaser coupling worked most efficiently on Ag(111) surfaces, as compared with Au(111) and Cu(111). The surface acts as a 2D supporting system that lets the molecules adsorb and orient in a plane, and may also mediate the reactions. The substitution pattern of the organic precursor molecules is also of great importance and simple steric shielding of the alkyne led to a suppression of side reactions. We believe that the approach presented herein is not restricted to the formation of π-conjugated linear chains but also allows for the formation of defined π-conjugated two-dimensional networks.

O 36.15 Tue 18:15 Poster B2

Nanoparticles droplets on a polymer brush studied by dissipative particle dynamics simulations — •Olga Guskova[1] and Christian Seidel[2] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

We use DPD simulations to investigate the self-assembly of nanoparticles (NPs) at a polymer brush/solvent (B/S) interface. Depending on the strengths of both the NP-solvent interaction and the NP-polymer one, NPs randomly distributed in solvent volume migrate to the polymer surface where they aggregate into droplets because of their solvophobic nature. We analyze the shape of the floating droplets as well as their effect on the free brush surface. In addition, the contact angles of NP droplets at the B/S interface are extracted from our simulations.

O 36.16 Tue 18:15 Poster B2

Clustering of adsorbed molecules on amorphous silica surfaces — •Yulia Rozhkova[1], Andrey Gurinov[1], Anna Orlova[2], Vladimir Maslov[2], Ilya Shenderovich[3], and Valentin Korotkov[1] — [1]St. Petersburg State University, St. Petersburg, Russia — [2]St. Petersburg National Research Institute on Information Technologies, Mechanics, and Optics, St. Petersburg, Russia — [3]University Regensburg, Germany

The specific current aim of this work is to inspect study the feasibility of spectral methods to characterize host-guest interactions and the dynamics of complex heterocycles loaded into silica pores of 4 to 20 nm in diameter. Acridine was adsorbed on the silica surface from vacuum and from solution. The strong hydrogen bound with proton shared is likely formed between hydroxyl groups and heteroatoms of acridine molecules in the first case. By comparing the luminescence spectra of acridine solution in the water and acridine adsorbed on silica from vacuum it was concluded that silica surface, dried in high vacuum at 420 K, contained a variety of adsorption centers, including adsorbed water. Adsorption of acridine from solution of dichloromethane results in formation of acridine aggregates on the surface. It can be happened in the case of island-type of adsorption. Acridine in dichloromethane solutions at different concentrations are investigated in detail. Concentration increasing was accompanied by formation of two types of aggregates. So, acridine self-aggregation was observed in solution. It may cause islet adsorption of acridine in the silica surface in the case of adsorption from solution.

O 36.17 Tue 18:15 Poster B2

Self-organized controlled positioning of nanoparticles in periodical arrays by horizontal dip coating — •Kathrin Kroth, Sabrina Darmawi, Limei Chen, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

With the help of a periodic array of cavities in the micrometer range, nanoparticles in colloidal particle suspension can be separated and arranged. The PMMA cavity structure is fabricated by EBL on a glass substrate. A drop of particle suspension, containing Au and polystyrene-latex particles (300nm), is deposited onto the array. Similar to standard dip coating, a second, motor-powered, plate slowly shoves the suspension above the structured surface. During this process the nanoparticles are arranged inside the cavities by the meniscus force. A characterization of the particles inside the cavities was carried out by SEM and Raman measurements. The Raman results will be discussed with respect to surface-enhancement effects of the signals.

O 36.18 Tue 18:15 Poster B2

***In Situ* Measurements of Protein Solutions with Nanoantenna Enhanced Infrared Spectroscopy** — •Robert Wolke[1], Jörg Bochterle[1], Frank Neubrech[1,2], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Fourier Transform Infrared spectroscopy (FT-IR) of aqueous solutions is a difficult task due to the strong absorption bands of water in the range of 1550-1750 cm^{-1} and 3000-3700 cm^{-1}. In order to enable measurements in transmission geometry, the thickness of the water layer should not exceed 10 μm. We created a microfluidic device (MFD) having nanoscopic metal rods inside the flow channel to utilize the signal enhancement seen in Surface-Enhanced Infrared Spectroscopy (SEIRS). This approach allows *in situ* SEIRS experiments in transmission geometry. Using photolithography, a flat microfluidic channel is inscribed on a calcium fluoride (CaF_2) wafer and closed off using a second CaF_2 wafer. SEIRS enhancement is achieved by micrometer long gold nanoantennas featuring localized surface plasmon resonance (LSPR) frequencies in the IR range. They are attached to the surface of the second wafer and can be exchanged easily. Our setup enables many new possibilities like *in situ* monitoring of protein binding kinetics to functional layers on the antennas or temperature dependent monitoring of protein conformation changes.

O 36.19 Tue 18:15 Poster B2

Investigation of surface plasmons on structured surfaces — •Tammo Böntgen[1], Jan Lorbeer[2], Marc Teichmann[2], Frank Frost[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Leibniz-Institut ür Oberflächenmodifizierung e.V., Permoserstr. 15, Leipzig, Germany

Nanoscale ripple pattern with a period of ≈90 nm were formed on SiO_2 surfaces by low-energy ion beam erosion ($E_{ion} < 2$ keV) at oblique ion incidence angles. The pattern was than coated with a gold film of ≈40 nm thikness. A Kretschmann configuration with a SiO_2 prism was used to allow surface plasmon excitation at the gold/air interface. Subsequently the sample was analyzed using a spectroscopic ellipsometer in the range from 370 nm - 1700 nm and angles of incidence (AOI) between 40° - 45°. This setup is similar to attenuated-total-internal-reflection readily used for study of surface plasmons. With this setup we were able to unravel a strong dependence of the surface plasmon resonance (SPR) frequency and strength on the in-plan orientation of the sample and the AOI. While the SPR is mostly independent of the in-plane orientation at AOI close to 45° a strong frequency shift with rotation is observed at smaller AOI. Similarly the strength of the SPR also changes with the in-plain orientation. In combination at 42° AOI a strong resonance at 860 nm is observed. This resonance vanishes if the sample is rotated by 90°.

O 36.20 Tue 18:15 Poster B2

Photothermal Microscopy in Liquid Crystals — •André Heber, Markus Selmke, Marco Braun, and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, D - 04103 Leipzig

A weakly fluorescent nano-particle that resonantly absorbs light dissipates its excitation energy into the environment as heat. The resulting temperature profile creates a refractive index profile around the particle which affects the scattering of a second off-resonant laser beam. This principle called photothermal contrast is used for correlation spectroscopy, imaging and absorption spectroscopy of absorbing nano-particles such as metallic nano-particles, quantum dots and single molecules.

Here we employ the technique to study single gold nano-particles in the uniaxial liquid crystal 8CB. It is anisotropic and has phase transitions at ambient temperature which are connected to large jumps in the refractive index. This can enhance the photothermal signal. But the signal depends sensitively on frequency and sample temperature due to the phase transition. The signal anisotropy can be used to measure the local orientation of nematic domains. We analyse the photothermal signal and model it analytically. The results show that photothermal microscopy is an ideal tool to study microscopic phase transitions.

O 36.21 Tue 18:15 Poster B2

Surface-enhanced infrared spectroscopy of CBP-molecules based on nanometer-sized gaps — •Christian Huck[1], Frank Neubrech[1,2], Andrea Toma[3], David Gerbert[1], Thomas Härtling[4], Enzo Di Fabrizio[3], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [3]Istituto Italiano di Tecnologia (IIT), Genova, Italy — [4]Fraunhofer Institute for Non-Destructive Testing, Dresden, Germany

Infrared spectroscopy is well suited for label-free characterization of molecular species. One disadvantage of the IR-spectroscopy is the relative low IR cross-section of molecular vibrations. One possibility to overcome this limitation is the use of surface-enhanced IR spectroscopy (SEIRS), where metal nanoparticles are used to enhance the electromagnetic field in their vicinity. If the resonance frequency of such particles matches molecule-vibrations, the vibrational signal can be enhanced up to 5 orders of magnitude. Additional enhancement is theoretically predicted and can be achieved by exploiting the extraordinary field enhancement of two antennas interacting across a very small gap.

Individual nanoantenna dimers with gap sizes down to 4 nm were prepared by electron beam lithography and subsequent photochemical metal deposition. Afterwards the dimers were covered with a 5 nm layer of CBP acting as a near-field probe. Our experiments show an increasing vibrational signal enhancement for decreasing gap sizes demonstrating the additional enhancement induced by nanometer-sized gaps.

O 36.22 Tue 18:15 Poster B2

Surface plasmon polariton induced effects onto the electronic transport through gold point contacts — •Philipp Nürnberger, Daniel Benner, Johannes Boneberg, Paul Leiderer, and Elke Scheer — Department of Physics, University of Konstanz, Germany

We study the impact of cw laser illumination onto the electronic transport through gold point contacts realized by Mechanically Controllable Break-junction (MCBJ) technique. For that purpose we excite surface plasmon polaritons at a grating, milled into the leads of the constriction. The excitation is controlled by an arrangement of additional gratings framing the constriction. Finally we compare the optical signal with the electronic response of the MCBJ.

O 36.23 Tue 18:15 Poster B2

Multicolor strong-field photoemission from metal nanotips — •Lara Wimmer, Georg Herink, Katharina Echternkamp, Daniel Solli, Sergej Yalunin, and Claus Ropers — Materials Physics Institute and Courant Research Centre, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We study strong-field photoemission from plasmonic nanotips driven by ultrashort laser pulses over a large spectral range. External static and optical fields enable us to control the photoemission process in a variety of ways. In multicolor scenarios, the cross-coupling of driving pulses at different wavelengths is investigated theoretically and experimentally, and the potential for ultrafast gating and steering of electrons in nanostructures is demonstrated.

O 36.24 Tue 18:15 Poster B2

Fabrication of plasmonic gold nanostructures for SERS using electron beam lithography and shadow evaporation — •Mario Fey — Justus-Liebig-Universität, Gießen, Deutschland

Plasmonic nanostructures exhibit a high local electric field and thus can be used for enhancing Raman signals. In order to fabricate such structures a combination of electron beam lithography (EBL) with a bilayer resist (PMMA on top of a copolymer) and shadow evaporation is used. Shadow evaporation is a means of overcoming the limitation of EBL by proximity effects and allows one to obtain metal structures with intermediate gaps of a few nanometers. A bilayer resist exhibits a pronounced T-bone undercut due to the different sensitivities of PMMA and the copolymer. The undercut allows one to carry out evaporation from different angles so the gap between two nanostructures can be tuned by the evaporation angle. The metallic line and dot structures with gaps of few nanometers were coated with dye solutions and studied by Raman spectroscopy to reveal plasmonic field enhancement in the Raman process.

O 36.25 Tue 18:15 Poster B2

Resonances and radiation patterns of metal-dielectric nanoantennas — •Manuel Gonçalves and Othmar Marti — Ulm University - Institute of Experimental Physics, Ulm, Germany

Plasmonic nanoantennas have been used to enhanced near-fields and scatter light emitted by small light sources at specific directions. However their radiation patterns are much more complex than classical antennas. Recently, materials of large refractive index were proposed for building antennas using the strong directivity of spectral well separated magnetic resonance modes. Silicon is one of the preferred candidates for such applications. On the other hand, destructive interferences between plasmonic radiant modes (bright plasmons) and subradiant modes (dark plasmons), as for magnetic dipoles and electric quadrupoles, in near-field coupled particles, leads to Fano resonances.

Using finite-element method (FEM) we study systems of plasmonic and dielectric particles presenting strong directivity, required for nanoantennas. We show how the Fano resonances can arise and their sensitivity on the particle size, environment and interparticle separation.

O 36.26 Tue 18:15 Poster B2

Polarization dependence of electron emission from cross-shaped nanoantennas — •Peter Klaer[1], Keno Krewer[1], Florian Schertz[1], Gerhard Schönhense[1], Hans-Joachim Elmers[1], Xiaofei Wu[2], and Bert Hecht[2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55122 Mainz — [2]Institut für Physik, Julius-Maximillians Universität Würzburg, 97074 Würzburg

Cross shaped nanoantennas that are designed to carry angular momentum have been fabricated by focused ion beam on single-crystalline gold flake. We show that these nanoantennas can be resonantly excited by femtosecond laser pulses using the emitted electron intensity from individual antennas, as determined by a photoemission electron microscope, as a measure for the plasmonic field enhancement. The resonant wavelength scales with the size of the antennas. The sample is illuminated from the front side at grazing incidence and from the backside at normal incidence. In both geometries the photoemission intensity of some antennas shows an unexpectedly pronounced polarization dependence, which can be explained by the actual shape of the nanoantennas.

O 36.27 Tue 18:15 Poster B2

Electromagnetic field distribution around gold nanorings under excitation with cylindrical vector beams — •Julia Fulmes[1], Christian Schäfer[1], Sebastian Jäger[2], Dominik A. Gollmer[1], Andreas Horrer[1], Dai Zhang[2], Alfred J. Meixner[2], Dieter P. Kern[1], and Monika Fleischer[1] — [1]Institute for Applied Physics, Eberhard Karls University of Tübingen, Germany — [2]Institute of Physical and Theoretical Chemistry, Eberhard Karls University of Tübingen, Germany

We investigate the optical behaviour of gold nanorings (NR) with variable geometries excited with cylindrical vector beams. The flexibility of lithographical fabrication processes enables precise control over the size, shape and surface smoothing of the nanostructures. We analyze the optical properties of gold nanorings by the combination of single particle dark field spectroscopy and confocal photoluminescence (PL) imaging. By illuminating the NR with cylindrical vector beams different photoluminescence patterns can be achieved depending on the ring diameters. The resulting PL images are explained by different overlap conditions between the ring and the individual components of the electromagnetic field in the focal spot. The observed excitation efficiency of discrete plasmon modes of the ring is in good agreement with numerical calculations. By matching the rings geometry to the illumination conditions the confined electromagnetic field can be maximized, enabling interesting applications of such nano-antenna as selective electric nanosource.

O 36.28 Tue 18:15 Poster B2

Numerical investigation of laser-triggered nanometer-sized

electron sources for ultrafast low-energy electron diffraction (ULEED) and ultrafast transmission electron microscopy (UTEM) — Stefanie Strauch, Simon Schweda, Max Gulde, Reiner Bormann, •Sascha Schäfer, and Claus Ropers — Materials Physics Institute and Courant Research Centre, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Sharp metallic tips excited by ultrashort laser pulses serve as promising electron sources for both UTEM and ULEED, due to their nanometer-sized emission area and large field enhancement at the tip apex. As part of the Göttingen UTEM initiative, we study the beam characteristics of pulsed Schottky field emitters within electron microscope geometries. In order to achieve optimal temporal and spatial pulse properties, it is crucial to understand the propagation of the photoemitted electron pulse in the beam-shaping electron optics for both high and low electron energy applications. We numerically investigate the electron optical design to improve the temporal pulse width, as well as the effective source size and beam emittance, and compare our findings with experimental results.

O 36.29 Tue 18:15 Poster B2

Surface plasmon travelling on a metallic stripe with nanometric constriction — •Golaleh Ghafoori, Daniel Benner, Johannes Boneberg, Paul Leiderer, and Elke Scheer — Department of Physics, University of Konstanz, Germany

We study the propagation of surface plasmons on a 4μm wide gold stripe of thickness 100nm by FDTD (Finite Difference Time Domain) simulations. For the excitation we use an optimized grating in the stripe. The surface plasmons propagate towards and across a constriction. We study the transmission over the constriction for different constriction shapes and as a function of the polarization. These studies allow the determination of local intensities in experiments with mechanically controllable break-junctions under light irradiation.

O 36.30 Tue 18:15 Poster B2

Probing the dispersion relation of surface plasmon polaritons by photoemission electron microscopy — •Jörn Willers Radke[1], Christoph Lemke[1], Till Leissner[1], Alwin Klick[1], Jacek Fiutowski[2], Kasper Thilsing-Hansen[2], Luciana Tavares[2], Jakob Kjelstrup-Hansen[2], Horst-Günter Rubahn[2], and Michael Bauer[1] — [1]Christian-Albrechts-Universität, IEAP, Kiel — [2]Syddansk Universitet, MCI, Sønderborg

We implemented two-photon photoemission electron microscopy (2P-PEEM) as a method to experimentally determine real and imaginary part of the dispersion relation of surface plasmon polaritons (SPPs) in the red and near-infrared spectral region. In the experiment a tunable Ti:Sapphire laser system is used for SPP excitation and detection via PEEM following an approach described in [1]. A characteristic periodicity in the photoemission data provide the relevant information on the real part of the SPP dispersion relation, the imaginary part is extracted from the decay length of the SPP signal. The validity of the approach is exemplified by measurements of the dispersion relation of SPPs propagating at the interface between a gold film and homogeneous films of para-hexaphenylene (p6P) at varying thickness. Furthermore, we also present experimental data of the SPP dispersion relation measured for individual dielectric loaded SPP waveguides. The example proofs the capability of this PEEM approach to provide a comprehensive view on SPP propagation properties in the frequency domain as governed by nanoscale objects.

[1] Kubo et al., Nano Lett. 7(2), p. 470 (2007)

O 36.31 Tue 18:15 Poster B2

Radiative heat transfer at the nanoscale between artificial structures — •Maria Tschikin[1], Philippe Ben-Abdallah[2], and Svend-Age Biehs[1] — [1]Carl von Ossietzky Universität, Institute of Physics, 26111 Oldenburg, Germany — [2]Carl von Ossietzky Universität, Institute of Physics, 26111 Oldenburg, Germany

The radiative heat flux for separation distances smaller than the thermal wavelength $\lambda_{\rm th} = \hbar c/(k_{\rm B}T)$ can be much larger than the black body limit due to the contribution of evanescent modes. Here we show that the inclusion of losses and evanescent contributions (in particular surface mode contributions) in the definition of the thermal conductance for photonic crystals is of fundamental importance. On the other hand we show that for hyperbolic materials like nanowire materials the dominant heat flux channel is provided by a broad band of frustrated modes rather than by surfaces modes. Finally, such artificial materials can be described by means of the effective medium theory in the long wavelength limit. We study the validity of the effective description for near-field radiation by comparing the effective calculation with exact results for layered media.

O 36.32 Tue 18:15 Poster B2

Single Molecule Junctions in Strong Optical Fields — •Hai Bi, Yuxiang Gong, Daniel Gerster, Joachim Reichert, and Johannes V. Barth — Physik Department E20, TUM, Garching

In order to advance the development of unimolecular electronic devices, it is mandatory to improve understanding of electron transport in single molecules, integrated in well-dependent environment. In this respect, multi-parameter studies are required to provide more information on such systems. Here we present a method which allows us to investigate single molecule junctions in strong optical fields. The molecules are self-assembled on a planar metal substrate and contacted by a gold-covered glass tip previously introduced for scanning near-field optical microscopy. The molecules are exposed to a photon flux guided through the tetrahedral tip that at the same time provides the electrical contact. The photon flux in the molecular junctions could be determined by photocurrent measurement of single photoactive proteins [1] and reveals significant field enhancements effects at the apex of the apertureless tip. This method can be employed to investigate a variety of nearly unexplored properties in single molecule junctions such as photoconductance and photocurrent generation and allows more over for an optical characterization of the molecular junctions by vibrational spectroscopic means as well.

[1] Daniel Gerster et al., Nature Nanotech. 7, 673-676 (2012)

O 36.33 Tue 18:15 Poster B2

Integration of a QCL in a SEIRA setup — •Anton Hasenkampf, Niels Kröger, Annemarie Annemarie Pucci, and Wolfgang Petrich — Kirchhoff-Institute for Physics Im Neuenheimer Feld 227 D-69120 Heidelberg

The main tool for surface-enhanced infrared absorption (SEIRA) for 60 years was the Fourier transform infrared (FTIR) spectrometer with a globar source. It allows spectroscopy of a sample with a spectral band width of 750 nm-100 000 nm. The disadvantage of this system is very low intensity of the used globar light source. This usually is compensated by long measurement times. In this work, we present an approach to combine a laser scanning microscopy setup with an external cavity quantum cascade laser (QCL) with grating in Littrow configuration. This enables a spectral measurement in the range of 7000 to 9000 nm. The 10^9 times higher spectral intensity compared to a globar can be used to reduce measurement time drastically and allows detection with a deuterated triglycine sulfate (DTGS). Since the spectral band width is limited, applications of the method are beyond broadband spectroscopy.

O 36.34 Tue 18:15 Poster B2

Ultrafast local dynamics of two-dimensional light modes — •David Leipold and Erich Runge — Institut für Physik, Technische Universität Ilmenau, Germany

The phenomenon of localization of waves by multiple coherent scattering attracts the interest of physical research for more than half a century. Anderson localization of matter waves is well established and a major building block of solid state physics. In contrast, the localization of classical waves – particularly light waves – is notoriously hard to observe and controversially discussed.

In this contribution, we present calculations considering the localized light field in ZnO nano-needle arrays. In particular, we investigate the influence of radiative losses on the formation of localized modes.

We compare results from numerical 2D solutions of Maxwells equations with open in-plane boundary conditions to 3D calculations including the finite needle-length and a rough substrate. The latter closely reproduce experimental findings[1] and have losses only in the out-of-plane directions. In the former, translational invariance in the out-of-plane directions suppresses these losses. Instead, losses in the in-plane directions are induced by open in-plane boundaries.

We find that modes showing mixed localized and lossy character form in the 2D case and can be distinguished by their lifetime and overlap with the vacuum region. These modes are similar to those found in the 3D calculations[1].

[1] M. Mascheck, *et al.*, Nature Photonics **6**, 293 (2012)

O 36.35 Tue 18:15 Poster B2

Observing the localization of light in space and time by ultrafast second-harmonic microscopy — M. Mascheck[1], S.

Schmidt[1], M. Silies[1], T. Yatsui[2], K. Kitamura[2], M. Ohtsu[2], •D. Leipold[3], E. Runge[3], and C. Lienau[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]School of Engineering, University of Tokyo, Japan — [3]Technische Universität Ilmenau, Germany

Anderson localization of light waves is notoriously hard to observe and controversially discussed for many decades. We present a method to investigate the degree of localization of the near-field of visible light in random arrays of vertically aligned ZnO nano-needles in space and time[1]. The second-harmonic emission of the needle array exhibits strong spatial fluctuations due to the presence of strong localization-induced hot-spots in the near-field intensity. We spatially resolve the second harmonic intensity with a tightly focused optical scanning-microscope setup.

In order to study the finite lifetime of the localized modes, the microscope is coupled to an interferometric frequency-resolved autocorrelation (IFRAC) setup. Combining both, the microscope focus and IFRAC with ultrashort laser pulses, we observe the localized light field with a spatial resolution better than 0.5μm and a temporal resolution better than 6 fs. We present measurements indicating hot-spot sizes smaller than the microscope resolution and mode lifetimes of 15 fs. In addition, 3D-FDTD calculations which are in well agreement with the experiment are presented[1].

[1] M. Mascheck *et al.*, Nature Photonics **6**, 293 (2012)

O 36.36 Tue 18:15 Poster B2

Simulation of antenna arrays for surface enhanced infrared spectroscopy — •Tobias W. W. Mass, Ann-Katrin U. Michel, Jon Mattis Hoffmann, and Thomas Taubner — 1st Institute of Physics, RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany

Metallic nanoantennas efficiently couple light into a region of subwavelength size. Antenna arrays designed for surface enhanced infrared spectroscopy (SEIRS) enable the detection of molecular vibration with high sensitivity [1]. Simulations are a useful tool to examine antenna coupling effects, which are crucial for plasmon resonance optimization [2]. Our simulation based investigations are concerned with square nanorod and hexagonal arranged triangle arrays having their plasmon resonances in the mid infrared region. Understanding the antenna coupling is important to predict the resonance position as well as the resonance width [3]. Therefore, analytic dipole approximations and numerical FDTD simulations are performed to explore the influence of coupling effects for different antenna lengths, array periodicities and substrate or cover material refractive indices. Experimental comparison is realized by FTIR measurements of e-beam and nanosphere lithography fabricated samples.

[1] Adato et al. *PNAS* **2009** 106(46), 19227-19232.

[2] Libermann et al. *Opt. Express* **2012** 20(11), 11953-11966.

[3] Adato et al. *Opt. Express* **2010** 18(5), 4526-4537.

O 36.37 Tue 18:15 Poster B2

Selective photo-induced metal deposition for fabrication of nanometer-sized gaps between infrared nanoantenna dimers — •Jochen Vogt[1], Frank Neubrech[1,2], Julia Katzmann[3], Thomas Härtling[3], Andrea Toma[4], Enzo Di Fabrizio[4], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Im Neuenheimer Feld 227, Heidelberg, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart, Germany — [3]Fraunhofer Institute for Non-Destructive Testing, Dresden, Germany — [4]Istituto Italiano di Tecnologia (IIT), Genova, Italy

Excited metallic nanostructures separated by gaps in the nanometer range exhibit high confinement of electromagnetic fields. Resonant in the infrared, they are well suited for Surface-Enhanced Infrared Spectroscopy (SEIRS) of adsorbed molecules. In the standard electron beam lithographic fabrication process, limitations due to secondary electron effects cause the gap sizes of the initial dimers to be not smaller than approximately 10nm. In our approach, we apply the method of photo-chemical metal deposition in order to achieve further gap narrowing. The gold dimers on the substrate are covered with a gold salt solution and exposed to a focused laser beam. In our sample design, unwanted lateral growth of the dimer arms is prevented by an organic film covering the dimers in such an alignment, that spatially selective photo-chemical growth is enabled. After the growth procedure, the shielding film was removed and IR spectroscopy to determine optical properties of the dimers as well as SEIRS measurements of organic molecules were performed.

O 36.38 Tue 18:15 Poster B2

Anomalous Light Scattering by a Charged Dielectric Particle — •Rafael Leslie Heinisch, Franz Xaver Bronold, and Holger Fehske — Institut für Physik, Universität Greifswald

We study for a dielectric particle the effect of surplus electrons on the anomalous scattering of light arising from the transverse optical phonon resonance in the particle's dielectric function. Excess electrons affect the polarizability of the particle by their phonon-limited conductivity, either in a surface layer (negative electron affinity) or the conduction band (positive electron affinity). We show that surplus electrons shift an extinction resonance in the infrared. This offers an optical way to measure the charge of the particle and to use it in a plasma as a minimally invasive electric probe.

O 36.39 Tue 18:15 Poster B2

Laser-triggered electron emission from a Schottky emitter assembly — •Reiner Bormann, Stefanie Strauch, Max Gulde, Simon Schweda, Sascha Schäfer, and Claus Ropers — Materials Physics Institute and Courant Research Centre, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Laser-triggered electron emission form sharp metal tips offers great potential for future pulsed high-brightness electron sources in ultrafast transmission electron microscopy (UTEM). However, their implementation in the advanced electron optics setup of an electron microscope is challenging. As part of the Göttingen UTEM initiative, we investigate the laser-induced electron emission characteristics of a Schottky emitter as utilized in commercial transmission electron microscopes. Specifically, we focus on the angular emission pattern and energy spread of the photoemitted electrons depending on the laser fluence, pulse duration and photon energy.

O 36.40 Tue 18:15 Poster B2

Ultrafast Photon and Electron Emission Induced at Nano-Structured Gold Tips — •Benjamin Schröder[1], Murat Sivis[1], Matthias Duwe[1], Philipp Kloth[2], Martin Wenderoth[2], and Claus Ropers[1] — [1]Materials Physics Institute and Courant Research Centre, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]IV. Physikalisches Institut, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Surface-plasmon-polaritons (SPPs) can be resonantly excited on metallic tapers by grating-coupling [1]. In this process, SPPs propagate towards the apex of the taper and converge in a localized hot spot with small nanometric dimensions. This type of evanescent apex excitation scheme provides a unique source for scanning probe applications at greatly reduced far-field background [2]. In this contribution, we study the excitation of SPPs on structured gold tips driven by broadband titanium:sapphire laser pulses. The spectral characteristics of the light emitted from the apex are evaluated as a function of angle of incidence, and a clear resonant behaviour is identified. We also examine nonlinear photoemission from such tips [3] and demonstrate that they are compatible with atomically resolving scanning tunnelling microscopy.

[1] C. Ropers et al., Nano Lett. 7, 2784 (2007)

[2] D. Sadiq, et al., Nano Lett. 11, 1609 (2011)

[3] R. Bormann, et al., Phys. Rev. Lett. 105, 147601 (2010)

O 36.41 Tue 18:15 Poster B2

Multi-photon photoelectron microscopy study of plasmonic silver structures and their interaction with porphyrin molecules — •Klaus Stallberg[1,3], Gerhard Lilienkamp[1], Herbert Pfnür[2,3], and Winfried Daum[1,3] — [1]Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover — [3]NTH School for Contacts in Nanosystems

Localized surface plasmons (LSPs) in metallic nanostructures provide strong field enhancement upon resonant irradiation with light of appropriate wavelength and thus strongly increase the efficiency of nonlinear optical processes such as multi-photon absorption. Moreover, previous studies in the frequency and time domain showed strong coupling of molecular excitations in light-absorbing molecules with surface plasmons of metallic surfaces and plasmonic nanostructures. In this contribution we apply energy-resolved photoelectron emission microscopy (PEEM) with short laser pulse excitation to study the role of plasmonic enhancement for two-photon photoemission from porphyrin molecular layers (Mg:TPP). As substrates for our experiments we use different silver structures epitaxially grown on Si(111)-(7x7) and

Si(100)-(2x1) substrates. Variation of the structure size allows for a tuning of the LSP resonance to match the absorption band of the porphyrin molecules. The effect of plasmonic enhancement in two-photon photoemission from these systems is studied in detail by variation of the photon excitation energy.

O 36.42 Tue 18:15 Poster B2

Theory for Multidimensional Coherent Spectroscopy of Plasmon Assisted Multi-Photon-Photoemission — Martin Aeschlimann[1], Tobias Brixner[3], Matthias Hensen[2], Christian Kramer[3], Pascal Melchior[1], Walter Pfeiffer[2], •Martin Piecuch[1], Christian Schneider[1], Christian Strüber[2], and Philip Thielen[1] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [3]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The recently demonstrated coherent 2D nanoscopy [1] allows for multidimensional coherent spectroscopy with sub-diffraction spatial resolution. In a first application the local hybridization of plasmon modes was investigated on a corrugated silver film [1]. The complete interpretation of multidimensional spectra requires a suitable model for the excitation process. Here we present a model for plasmon assisted multiphoton photoemission in which both, collective and single particle excitations are treated as quantum excitations. Based on this, coherent 2D spectra are simulated and the concept of phase cycling is applied to identify particular quantum mechanical pathways through an appropriate linear combination of detectable photoemission signals. The resulting two dimensional photoemission spectra grant direct access to the coupling parameter of the system under investigation.

[1] Aeschlimann et al., *Science* 333 (6050), 1723-1726 (2011)

O 36.43 Tue 18:15 Poster B2

Light intensity modulation in tailored magneto-plasmonic crystals by a novel longitudinal magneto-photonic effect — V.I. Belotelov[1,2], L.E. Kreilkamp[3], •M. Jäckl[3], I.A. Akimov[3], A.N. Kalish[1,2], D.A. Bykov[4], S. Kasture[5], Achanta Venu Gopal[5], M. Nur-E-Alam[6], M. Vasiliev[6], L.L. Doskolovich[4], D.R. Yakovlev[3], K. Alameh[6], A.K. Zvezdin[2], and M. Bayer[3] — [1]Lomonosov Moscow State University, 119991 Moscow, Russia — [2]Prokhorov General Physics Institute, Russian Academy of Sciences, 119991 Moscow, Russia — [3]Experimental Physics 2, TU Dortmund University, D-44221 Dortmund, Germany — [4]Image Processing Systems Institute, Russian Academy of Sciences, 443001 Samara, Russia — [5]Tata Institute of Fundamental Research, 400005 Mumbai, India — [6]Electron Science Research Institute, Edith Cowan University, 6027 Joondalup, WA, Australia

We present our study on a novel magneto-optical phenomenon observed in a hybrid metal-dielectric structure consisting of a one-dimensional gold grating on top of a magnetic waveguide layer. When a magnetic field is applied perpendicularly to the grating slits the field distribution of its optical modes and thus the mode excitation conditions are changed. Under those conditions two principal modes of the magnetic layer – TM- and TE-modes – acquire additional field components and thus turn into quasi-TM and quasi-TE-modes, respectively. In the optical far-field this modification of the modes manifests itself in the distinct alteration of the optical transmission or reflection coefficients when the structure becomes magnetized.

O 36.44 Tue 18:15 Poster B2

Dark-field spectroscopy and simulation of plasmonic modes in single nanostructures — •Andreas Horrer, Christian Schäfer, Dominik A. Gollmer, Julia Fulmes, Dieter P. Kern, and Monika Fleischer — Institute for Applied Physics, Eberhard Karls University of Tuebingen, Auf der Morgenstelle 10, 72076 Tuebingen, Germany

Due to their strongly localized electrical fields and sharp resonances in the optical or infrared range, plasmonic nanostructures provide a promising platform for many applications, for example the detection of molecules with high sensitivity. For such applications it is crucial to be able to fabricate structures with well-defined sizes and shapes in a controlled manner and to understand their plasmonic resonances. Dark-field spectroscopy, where scattered light from individual nanoparticles can be detected in the far field, is a highly useful method for the study of the plasmonic modes of such structures. Different plasmonic nanostructures like gold nanocones, nanotriangles or nanodiscs were fabricated with varying sizes and aspect ratios and the optical properties of single structures were investigated by dark-field spectroscopy. For the characterization of the plasmonic modes of the nanostructures the spectra were compared to the results of finite element method based simulations of the structures in differently polarized electromagnetic fields. An overview over different structures, their spectral properties and corresponding numerical simulations will be presented.

O 36.45 Tue 18:15 Poster B2

ToF-PEEM for Probing and Control of Nanoplasmonic Optical Fields at Ultrahigh Spatiotemporal Resolutions — •Soo Hoon Chew[1,2], Alexander Gliserin[1,2], Matthias Kübel[2], Huanglei Bian[1], Kellie Pearce[1,2], Christian Späth[1], Florian Schertz[3], Jürgen Schmidt[1], Matthias Kling[2], and Ulf Kleineberg[1] — [1]Faculty of Physics, Ludwig Maximilian University of Munich, Germany — [2]Max Planck Institute of Quantum Optics, Germany — [3]Institute of Physics, University of Mainz, Germany

The attosecond plasmonic field microscope was developed to study the plasmonic dynamics in nanostructured surfaces with attosecond temporal and nanometer spatial resolution. We obtained a spatial resolution of 200 nm from imaging the gold nanostructures using time-of-flight-photoemission electron microscopy (ToF-PEEM) in combination with extreme ultraviolet attosecond pulses from a high harmonic generation source. We find that energy-filtered imaging could reduce the chromatic aberrations and the primary electrons are not affected by the space charge problem. Recently, strong carrier-envelope phase (CEP) effects are shown to be important in controlling electron motion in the matters. In order to investigate and control CEP effects on plasmonic nanostructures for every single laser shot, the phase-tagged ToF-PEEM has been developed. First experiments measuring CEP dependence on single gold nanoparticles have been performed with 10 kHz few-cycle laser pulses. These experiments demonstrate first steps toward the temporal characterization and CEP control of nanoplasmonic fields in a femtosecond optical-pump/attosecond XUV-probe scheme.

O 36.46 Tue 18:15 Poster B2

Spatiotemporal characterisation of nanofabricated silver plasmonic waveguides using 2P-PEEM — •Kellie Pearce[1,2], Christian Späth[1], Soo Hoon Chew[1,2], Sebastian Nobis[1], Anika Spreen[1], Jürgen Schmidt[1], and Ulf Kleineberg[1] — [1]Department of Physics, Ludwig Maximilian University of Munich, Garching, Germany — [2]Max Planck Institute of Quantum Optics, Garching, Germany

We characterise the static and dynamic properties of plasmonic waveguides and nanostructures using two-photon photoemission electron microscopy (2P-PEEM). The influence of the size, shape, and length of nanolithographically fabricated silver arrow-like waveguides on the surface plasmon excitation, propagation and focussing is investigated. In addition, we examine the polarization dependence of hotspots in coupled structures such as silver bow ties and chemically-synthesised gold nanospheres. Characterisation is performed as a first step towards time-resolved measurements using 10kHz few-cycle laser pulses.

O 36.47 Tue 18:15 Poster B2

Calculation of gold nanoparticle-enhanced up-conversion intensity of Er^{3+} ions — •Deepu Kumar[1], Florian Hallermann[1], Stefan Fischer[2], Alexander Sprafke[3], Jan Christoph Goldschmidt[2], and Gero von Plessen[1] — [1]Intitute of Physics (1A), RWTH Aachen University, 52056 Aachen, germany — [2]Fraunhofer ISE, Heidenhofstr. 2, 79110 Freiburg, Germany — [3]μMD Group, Institute of Physics, Martin-Luther University Halle-Wittenberg, 06120 Halle, Germany

The current generation process in conventional solar cells does not have any contribution from photons with energies lower than the silicon band gap (1.12 eV). Up-conversion processes, such as the excitation of electrons via sequential absorption of infrared photons in rare-earth ions, may be suited to exploit the near-infrared region of the solar spectrum. These processes lead to the conversion of two or more photons with low energy into one sufficiently high-energy photon that can be absorbed in silicon. We calculate the intensity enhancement of the up-conversion photoluminescence from a thin planar layer of Er^{3+} ions induced by a nearby gold nanosphere. We discuss the roles of the various excitation and decay processes involved in this enhancement.

O 36.48 Tue 18:15 Poster B2

Fabrication and investigation of plasmonic nano gratings

for photovoltaic devices — •Felicitas Walter, Dominik A. Gollmer, Christopher Lorch, Jiri Novak, Frank Schreiber, Dieter P. Kern, and Monika Fleischer — Institute for Applied Physics, Eberhard Karls University, 72076 Tübingen, Germany

The emerging field of plasmonics has brought about methods for guiding and localizing light at the nanoscale. Now the attention of researchers in this field has turned towards applications, where design approaches based on plasmonics can be used e.g. to improve absorption in photovoltaic devices. In this context we combine organic photovoltaics with plasmonic gold structures. It is our goal to increase the efficiency of such devices by the optical near field enhancement and scattering at the structured interfaces. Plasmonic gold structures are fabricated using the serial procedure of electron beam lithography, with which we have great flexibility regarding size and shape. First line gratings were fabricated, where we varied the periodicity and the line width. In addition, dot gratings with varying radii and periodicity were produced. For testing these gratings can be covered with organic layers relevant for photovoltaics. The optical properties of the structures are studied without and with such layers. Here we will present scanning electron micrographs of the gold structures and optical transmission spectra of these structures without and with added organic thin films.

O 36.49 Tue 18:15 Poster B2

Fabrication of nanoscaled plasmonic structures for Photoelectron emission microscopy (PEEM) by electron beam lithography — •Christian Späth, Anika Spreen, Soo Hoon Chew, Kellie Pearce, and Ulf Kleineberg — Ludwig-Maximilians-Universität München, Department für Experimentalphysik und Laserphysik, Coulombwall 1, 85748 Garching

To support experiments in the field of ultrafast nano-optics and plasmonics the fabrication of metallic nanostructures of various sizes and shapes by electron beam lithography is an important prerequisite.

We report on our latest results in the development process of nanoantennas for local optical field enhancement by localized surface plasmons (LSP) and tapered plasmonic waveguides for transportation and possible control of surface plasmon polaritons (SPP). Waveguides with different geometries with respect to size, tip shape, incoupling grating periods have been written in PMMA bilayer resist systems on Si (100) wafer and have subsequently been metal coated with ultrathin Ag or Au layers and finalized by lift-off; similarly with all nanoantennas, e.g. bow ties, ellipsoids and gratings in different sizes and arrangements.

The topography of these structures has been analyzed by means of atomic force and scanning electron microscopy and the spatiotemporal plasmonic properties of the nanosamples have been investigated by nonlinear laser photoelectron emission microscopy. Furthermore we plan to utilize different substrate materials such as diamond like carbon (DLC) or indium zinc oxide (InZnO) to improve image contrast during PEEM experiments.

O 36.50 Tue 18:15 Poster B2

Infrared spectroscopy of phase transitions in metal nanosystems — •Fabian Hötzel[1], Chung Vu Hoang[1,2], Tadaaki Nagao[2], Robert Lovrinčić[1,3], and Annemarie Pucci[1] — [1]Kirchhoff Institute of Physics , Heidelberg University, Heidelberg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan — [3]Weizman Institute of Science, Rehovot, Israel

Metals show strong plasmonic effects in the infrared, which enables contact-free conductivity studies. Contribution from relaxation processes and band structure can be separately derived from spectral information. Even more, polarization dependent studies may reveal anisotropic behaviour. We present and explain examples with phase transitions as such between different metallic structures and a Peierls-type transition. This contribution is related to DFG-FOR 1700.

O 36.51 Tue 18:15 Poster B2

Characterization of Horizontally-aligned Carbon Nanotubes: Impact of Tip-induced Strain and Bias Voltage — •Parisa Bayat[1], Raul D. Rodriguez[1], Alexander Villabona[1], Sascha Hermann[2], Stefan E. Schulz[2], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, TU Chemnitz — [2]ZfM, TU Chemnitz

Carbon nanotubes (CNTs) have attracted huge attention in the area of nanotechnology since the seminal work of Iijima in 1991. Several interesting examples of the advantages of CNTs like their high carrier mobility, remarkable thermal conductivity and significant mechanical strength have been demonstrated. The focus of this work is on the electrical properties of semiconducting single wall CNTs (SWCNTs) horizontally aligned between two pre-structured palladium electrodes in a field-effect transistor configuration. In this work we aim at investigating the role of tip-induced deformation of the SWCNTs by the AFM tip and the effect of bias voltage. Atomic force microscopy (AFM) in force spectroscopy mode, current sensing AFM, Kelvin force microscopy, and (tip enhanced) Raman spectroscopy are employed for the characterization. It was reported that the band structure of a carbon nanotube can be dramatically altered by mechanical strain reflected in examples such as the metallization of SWCNT by locally applying pressure. Theoretical works predict that band gap changes can range between +/-100 meV per 1% stretch, depending on CNT chirality. Our work aims at evaluating and verifying these predications. DFG-Research Unit 1713 "Sensoric Micro- and Nanosystems" SMINT is acknowledged for financial support.

O 36.52 Tue 18:15 Poster B2

Characterisation of Boron-doped Silicon Nanowires — •Stefan Weidemann[1], Peter Schäfer[2], Stefan Kowarik[2], Klaus Rademann[3], and Saskia F. Fischer[1] — [1]Novel Materials, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Coherent Optics with X-rays, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [3]Nanostructured Materials, Humboldt-Universität zu Berlin, 10099 Berlin, Germany

Nanostructures of silicon reveal new intrinsic properties like decreased thermal conductivity [1]. To date, it remains a challenge to measure simultaneously thermal and electronic transport properties of individual silicon nanowires. Here, we prepare silicon nanowires by metal-assisted chemical etching (MACE)[2] with solid, rough and porous surfaces in dependence of the boron doping concentration (resistivities of $\rho <10$ mΩcm, ρ =14-23 Ωcm, $\rho >1$ kΩcm).

Nanowire lengths up to 110 μm (undoped Si, $\rho >1$ kΩcm), 90 μm (medium doped Si, ρ=14-23 Ωcm) and about 30 μm (highly doped Si, ρ<10 mΩcm) are achieved. Fabrication on wafer scale is possible. Surface and structural properties of both nanowire ensembles and individual nanowires are investigated by electron microscopy and x-ray diffraction. Single nanowires are investigated with respect to their thermoelectrical properties.

[1] A. I. Hochbaum *et al.*, Nature 451, 163 (2008)
[2] Z. Huang *et al.*, Adv. Mater. 2011, 23, 285-308

O 36.53 Tue 18:15 Poster B2

Mesoporous Silicon Nanowire Characterisation by Nitrogen Gas Adsorption — •Stefan Weidemann[1], Dirk Wallacher[2], and Saskia F. Fischer[1] — [1]Novel Materials, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department Sample Environments, Helmholtz-Zentrum Berlin, 14109 Berlin, Germany

Silicon nanowires produced by metal-assisted chemical etching have different surface morphologies in dependence of the doping concentration[1]. Solid, rough and porous nanowire surfaces can be prepared. While the formation mechanism of rough surfaces is still unclear we investigate the surface texture of mesoporous silicon nanowires by nitrogen gas adsorption.

We fabricated silicon nanowire ensembles of undoped Si (resistivity ρ>1 kΩcm), medium boron doped Si (ρ=14-23 Ωcm) and highly boron doped Si (ρ<10 mΩcm) and determined surface properties like pore diameter, pore volume and sample surface area. We discuss for samples of different preparation parameters such as etching time and etchant concentration how the pore formation is affected and determine the mean poresize distribution on highly doped nanowires.

[1] A. I. Hochbaum *et al.*, Nano Lett., Vol. 9, No. 10, 2009

O 36.54 Tue 18:15 Poster B2

Scanning tunneling microscopy of reconstructions including nanoline structures on the SrTiO$_3$(001) surface — •Ines Weidle, Jochen Settelein, Julian Aulbach, Jörg Schäfer, Michael Sing, Lenart Dudy, and Ralph Claessen — Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

The surface of cleaved SrTiO$_3$ hosts a two-dimensional electron gas which has recently attracted much attention as a model system for low-dimensional metals. On the other hand the surface of this oxide is known to exhibit a multitude of reconstructions. Among these reconstructions produced by a sequence of sputtering and annealing cycles, there are self-assembled nanoline-like structures of reduced titanate. These nanowires may have potential interest for (quasi-) one-dimensional physics of the electronic structure. We have explored the fabrication of these reconstructions on Nb-doped SrTiO$_3$ and present our scanning tunneling microscopy (STM) measurements on nanoline structures.

A systematic study of the evolution of the various reconstructions has been performed as a function of the annealing treatment. After annealing, the STM images show widespread formation of a c(4 × 2) reconstruction. Subsequent annealing treatment promotes the occurrence of so-called dilines in (6 × 2) reconstruction. Their density can be increased upon further temperature treatment. The presentation discusses the various surface phases observed and provides a comparison with the pertinent literature.

O 36.55 Tue 18:15 Poster B2

Polystyrene spheres assisted anodization method for the preparation of size-controlled pore diameter and separation in the AAO template — •Yaoguo Fang[1], Kin Mun Wong[1], Liaoyong Wen[1], Yan Mi[1], Gerhard Wilde[2], and Yong Lei[1] — [1]H1107 Heliosbau, Technische Universität Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany — [2]Heisenbergstr. 11 48149 Münster, Germany

Abstract We propose a method where the size of the pores in the anodic aluminum oxide (AAO) template can be precisely controlled with the use of the regular arrays of polystyrene (PS) spheres as a mask. A monolayer of PS spheres was first prepared on the bare aluminum foil and the silica sol was introduced into the spaces between the PS spheres. This was followed by removing the PS spheres with toluene and consequently highly ordered arrays of micro-bowl structures are fabricated on the Al foil. With the use of the PS spheres, the center of the bowl structures on the Al surface are not covered by the silica gel due to contact between the bottom of the PS sphere and the Al surface during the silica sol infiltration. With the use of the PS spheres, most of the Al surface will be covered by the silica sol and the pores can only be formed at the center of highly ordered arrays of micro-bowl structures by the normal two-step anodization procedure. Importantly, with the use of the smaller PS spheres, smaller pore diameters (less than 10 nm) in the AAO template can be obtained. In addition, the separation between the pores can be adjusted with the different sizes of the PS spheres.

O 36.56 Tue 18:15 Poster B2

Polystyrene spheres assisted anodization method for the preparation of size-controlled pore diameter and separation in the AAO template — •Yaoguo Fang[1], Kin Mun Wong[1], Liaoyong Wen[1], Yan Mi[1], Gerhard Wilde[2], and Yong Lei[1] — [1]H1107 Heliosbau, Technische Universität Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany — [2]Institut für MaterialPhysik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Abstract We propose a method where the size of the pores in the anodic aluminum oxide (AAO) template can be precisely controlled with the use of the regular arrays of polystyrene (PS) spheres as a mask. A monolayer of PS spheres was first prepared on the bare aluminum foil and the silica sol was introduced into the spaces between the PS spheres. This was followed by removing the PS spheres with toluene and consequently highly ordered arrays of micro-bowl structures are fabricated on the Al foil. With the use of the PS spheres, the center of the bowl structures on the Al surface are not covered by the silica gel due to contact between the bottom of the PS sphere and the Al surface during the silica sol infiltration. With the use of the PS spheres, most of the Al surface will be covered by the silica sol and the pores can only be formed at the center of highly ordered arrays of micro-bowl structures by the normal two-step anodization procedure. Importantly, with the use of the smaller PS spheres, smaller pore diameters (less than 10 nm) in the AAO template can be obtained. In addition, the separation between the pores can be adjusted with the different sizes of the PS spheres.

O 36.57 Tue 18:15 Poster B2

Polystyrene spheres assisted anodization method for the preparation of size-controlled pore diameter and separation in the AAO template — •Yaoguo Fang[1], Kin Mun Wong[1], Liaoyong Wen[1], Yan Mi[1], Gerhard Wilde[2], and Yong Lei[1] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & IMN MacroNano (ZIK), Institute for Physics and IMN MacroNano (ZIK),Technische Universität Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany — [2]Institut für MaterialPhysik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

We propose a method where the size of the pores in the anodic aluminum oxide (AAO) template can be precisely controlled with the use of the regular arrays of polystyrene (PS) spheres as a mask. A monolayer of PS spheres was first prepared on the bare aluminum foil and the silica sol was introduced into the spaces between the PS spheres. After removing the PS spheres, highly ordered arrays of micro-bowl structures are fabricated on the Al foil. With the use of the PS spheres, the center of the bowl structures on the Al surface are not covered by the silica gel due to contact between the bottom of the PS sphere and the Al surface during the silica sol infiltration. Therefore most of the Al surface will be covered by the silica sol and the pores can only be formed at the center of highly ordered arrays of micro-bowl structures by the normal two-step anodization procedure. Importantly, with the use of the smaller PS spheres, smaller pore diameters(less than 10nm)in the AAO template can be obtained. In addition, the separation between the pores can be adjusted with the different sizes of the PS spheres.

O 36.58 Tue 18:15 Poster B2

New approach to the fabrication of ssDNA/oligo(ethylene glycol) monolayers and complex nanostructures — •M Nuruzzaman Khan[1], Vinalia Tjong[2], Ashutosh Chilkoti[2], and Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Department of Biomedical Engineering, Duke University, N C 27708-0300, USA

Immobilization of single stranded DNA (ssDNA) on solid support is an important issue for binding and detection of the complementary DNA target as well as for the recognition of DNA binding proteins. Here we present a universal two-step approach to fabricate mixed monomolecular films comprising thiolated ssDNA and oligo(ethylene glycole) substituted alkanethiolates (OEG-AT) which exhibit biocompatible properties providing a suitable matrix for the ssDNA . At first, the primary OEG-AT monolayer was irradiated with electrons to create defects in a controlled fashion. In the second step, a defect-promoted exchange between the molecules in the monolayer and ssDNA species in solution occurred, with the extent depending on the irradiation dose. The approach was combined with E-beam lithography, which allowed us to fabricate versatile ssDNA patterns of any required shape imbedded in the protein-repelling matrix. Further, applying surface initiated enzymatic polymerization, we succeeded to amplify the above ssDNA/OEG-AT patterns in the z-direction in a controlled fashion. Both ssDNA pattern and related 3D nanostructures can be widely used as versatile nanofabrication platform in such important fields as bio-engineering, bio-technology, and sensor fabrication.

O 36.59 Tue 18:15 Poster B2

Fabrication of iron nanostructures on various surfaces via focused electron beam induced processing in UHV — •Fan Tu, Florian Vollnhals, Martin Drost, Esther Carrasco, Matthias Franke, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr.3, D-91058, Erlangen, Germany

Focused electron beams are well suited to manipulate matter on the nanoscale. In our 'surface science approach' to focused electron beam induced processing (FEBIP) we either deposit fragments of adsorbed precursor molecules or directly change the properties of a substrate itself. With the focused electron beam induced surface activation (EBISA) we recently explored a novel technique in which oxide surfaces, e.g. of SiOx and TiO2 substrates can be chemically activated on the nanoscale after local electron beam irradiation [1,2]. These activated region can be later on developed with Fe(CO)5 resulting in pure iron nanostructures. With this contribution we considerably expand the EBISA technique to adsorbed organic films on metal substrates and well-defined oxide reconstructions both on metal substrates. This work was supported by the DFG via grant MA 4246/1-1.

[1] M.M. Walz et al., Angw. Chem. Int. Ed., 49 (2010), 4669;
[2] M.M. Walz et al., Appl. Phys. Lett., 100(2012), 053118

O 36.60 Tue 18:15 Poster B2

Quantum-Well-States with non-vanishing momentum component in Cu/Co/Cu(100)-Systems — Philipp Kloth, Martin Wenderoth, •Philip Willke, Henning Prüser, and Rainer G. Ulbrich — IV. Phys. Inst., Georg-August-Universität, Göttingen

Quantum-well-states can form in metallic heterostructures and have been investigated by several methods, for example photoemission [1] and STM [2]. We report the formation of quantum-well-states above the Fermi energy for a Cu/Co/Cu(100)-layer system using low-temperature scanning tunneling spectroscopy. These states emerge from a stationary point at the Fermi surface with a non-zero parallel momentum component. We show that the preparation method of the metallic heterostructures is a crucial parameter for the formation of these states. By comparing our results with a transfer matrix simulation in combination with a tight-binding band structure calculation, a cross-over between resonance states and bound states can be identified. This results in a phase shift of the energetic dispersion of these states with varying the confinement thickness. Furthermore, these states seem to dominate the density of states of copper compared to the more prominent well-states in this system with no parallel wave vector component.

We acknowledge the financial support by the DFG SFB 602 Project A3.

[1] J.E. Ortega, F.J. Himpsel, G.J. Mankey, and R.F. Willis, Phys. Rev. B 47, 1540-1552 (1993)

[2] M. Becker and R. Berndt, Phys. Rev. B 81, 205438 (2010)

O 36.61 Tue 18:15 Poster B2

PTCDA adsorption on KCl and NaCl(100) surfaces studied from first principles — •Hazem Aldahhak, Wolf Gero Schmidt, and Eva Rauls — Theoretische Physik, Universität Paderborn

In recent years, various highly regular supramolecular architectures of self-organized molecules on crystals have been designed and used in the bottom-up device technology.

In the past, metal surfaces have frequently been used as substrate. However, metal substrates induce screening and quenching effects and thus hamper the detailed spectroscopy of the adsorbed overlayer. In contrast, molecular adsorption on ionic crystals like sodium or potassium chloride opens the possibility to study electronically decoupled molecules.

Here we present density-functional theory calculations on the adsorption of PTCDA on KCl and NaCl (100) surfaces. Thereby the adsorption on flat surfaces as well as stepped substrates steps is investigated. Experimentally, both flat-lying (P-type) as well as standing molecules (S-type) are observed depending on the preparation conditions. In order to understand and rationalize the adsorption mechanisms leading to the formation of these structures, a large variety of interface geometries was studied and analyzed with respect to the contribution of ionic, covalent and van-der-Waals interactions between adsorbates and substrates. The influence of the substrate and bonding mechanism on the molecular electronic structure is investigated in detail and compared with the experimental data available.

O 36.62 Tue 18:15 Poster B2

Irradiation of graphene on calcium fluoride with highly charged ions — •Philipp Ernst, Jakob Krämer, Roland Kozubek, Johannes Hopster, and Marika Schleberger — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

We have irradiated CaF_2 and graphene on CaF_2 with slow (E_{kin}=260 keV) highly charged ions ($^{129}Xe^{35+}$), which leads to defects on the surface in the nm-range. The topography of the sample is analyzed using an atomic force microscope (AFM) in contact- and tapping-mode. Two different types of masks were designed to compare irradiated areas on CaF_2 with unirradiated areas. Thus, it is possible to distinguish between small clusters most likely due to sputtering and defects directly created by HCI impact. We show, that AFM operating parameters have to be carefully chosen to perform a quantitative analysis of irradiation induced defects. The uncovered CaF_2 surface shows the well known hillocks induced by individual HCI impacts. The defects on graphene appear as regions of increased friction. By flipping the graphene flake with the AFM tip, the CaF_2 substrate below could be studied. There, the diameter of the hillocks are significantly smaller (7-8 nm) than on the uncovered sections of CaF_2 (15-40 nm).

O 36.63 Tue 18:15 Poster B2

Electronic characterization and ion induced modification of single layer MoS2 sheets — •Kolyo Marinov[1], Oliver Ochedowski[1], Nils Scheuschner[2], Ulrike Hutten[1], Janina Maultzsch[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Duisburg, Germany — [2]Technische Universität Berlin, Berlin, Germany

Ultrathin sheets of layered transition metal dichalcogenides like MoS2 have drawn much interest recently. While graphene lacks a band gap which complicates its integration in future semiconducting devices, MoS2 shows a transition from an indirect towards a direct band gap semiconductor in the case of single layer MoS2 sheets. It has already been demonstrated that the electron mobility matches Si and high on/off ratios of MoS2 devices can be achieved. We will present Kelvin probe force microscopy and *-photoluminescence data of single layer MoS2 exfoliated on SrTiO3. Our data shows a possible charge transfer and shift in the work function induced by the substrate. Furthermore, it will be shown how swift heavy ion irradiation can be used to taylor thin MoS2 sheets by creating rifts in the MoS2 sheet along the ion trajectory or creating folded MoS2 sheets which exhibit closed bilayer edges.

O 36.64 Tue 18:15 Poster B2

Automated spray coating process for the synthesis of extensive artificial opals — •Daniela Schneevoigt[1], Alexander Sprafke[1], and Ralf Wehrspohn[1,2] — [1]Martin-Luther-Universität, Halle-Wittenberg, Deutschland — [2]Fraunhofer IWM, Halle, Deutschland

3D photonic crystals such as artificial opals are a promising material class for the use in advanced light management concepts for solar cells [1]. To be able to integrate such concepts within the photovoltaic industry a low-cost and large-scale technique to produce photonic crystals of high quality is needed.

Here, we report on the successful implementation of an automated process for a spray induced self-assembly of 3D artificial opals. In contrast to previous work, non-porous substrates, such as glass or Si wafers are used. To achieve artificial opals of high quality, process parameters such as the solid content of the dispersion, the substrate material and the dispersion agent have to be adjusted. Most important is the understanding of the drying process, which is strongly affected by the choice of the aforementioned parameters. Therefore an extensive investigation of the influence of these parameters on the spray coating process was carried out in order to achieve a more precise understanding of the crystallization mechanism and to gain a better control over the fabrication process of artificial opals by spray coating.

[1] Sprafke, A., Wehrspohn, R., Light trapping concepts for photon management in solar cells. Green, 2(4): 177-187, (2012).

O 36.65 Tue 18:15 Poster B2

Are there coherent phonon signatures of a photoinduced, meta-stable state in *1T*-TaS_2? — •Manuel Ligges[1], Simon Freutel[1], Isabella Avigo[1], Ljupka Stojchevska[3], Laurenz Rettig[1], Tomaz Mertelj[3], Ping Zhou[1], Dragan Mihailovic[3,4], Lutz Kipp[2], Kai Rossnagel[2], and Uwe Bovensiepen[1] — [1]Univ. Duisburg-Essen, Germany — [2]Christian-Albrechts-Univ. zu Kiel, Germany — [3]Complex Matter Dept., Jozef Stefan Institute, Ljubljana, Slovenia — [4]CENN Nanocentre, Ljubljana, Slovenia

1T-TaS_2 is a layered transition metal-dichalgoenide that exhibits a manifold of electronic and structural phases, giving rise to a complex interplay between electronic correlation effects and structural modifications. Of particular interest is the photo-induced melting of the Mott-Hubbard phase that is associated with a partial removal of commensurate charge-density wave (CCDW) order. We performed pump-probe photoemission experiments in which coherent phonon signatures associated with the amplitude mode of this CCDW are observed. Upon strong (a few mJ/cm^2) infrared few-pulse pre-excitation of the material before the pump-probe experiments, severe changes in the vibrational spectrum can be observed that persist on very long timescales (> hrs). The signature observed before this intense excitation (2.4 THz) splits up into a 2.4 THz and a 2.5 THz component with comparable amplitude. We will discuss meta-stable configurations of the CCDW ordered state as a potential origin of this observation. We acknowledge financial support by the Deutsche Forschungsgemeinschaft through BO 1823/2, /4 and the European Union under grant agreement 280555 within FP7.

O 36.66 Tue 18:15 Poster B2

Microscopic and spectroscopic studies of epoxy-steel interfaces — •Henning Munkert[1], Lienhard Wegewitz[1,2], Florian Voigts[3], Heinz Palkowski[2,4], and Wolfgang Maus-Friedrichs[1,2] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal — [2]Clausthaler Zentrum für Materialtechnik, TU Clausthal — [3]Institut für Elektrochemie, TU Clausthal — [4]Institut für Metallurgie, TU Clausthal

Deformable sandwich sheet materials produced as raw materials and formed afterwards to complex geometries require a good bonding to guarantee a stable shear transfer between the single layers. However, due to the deformation, failures by delamination often occur between the epoxy and the metal. The aim of our work is to understand the basic effect of the interfaces' bonding behavior in selected preparation steps of the system. It is shown how surfaces change topographically as well as in their chemical composition, if epoxy and steel layers get into contact with each other: The interaction between the two materials results in various functional carbon groups like C-C, C-O and C=O and in the reduction of iron according to the different preparation steps. These effects are studied with Atomic Force Microscopy (AFM) and X-ray Photoelectron Spectroscopy (XPS).

O 36.67 Tue 18:15 Poster B2

Surface alteration during the corrosion of sodium silicate glasses — •Melanie Dathe and Hans Roggendorf — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik

The dissolution of sodium silicate glasses is a standard method for the production of soluble glass (waterglass). Therefore, the processes of the dissolution of sodium silicate glasses are investigated. The composition of the sodium silicate glasses investigated here was $Na_2O \cdot x\ SiO_2$, with x=2 and 3.3. The dissolution of the glass can be regarded as an extreme case of glass corrosion. During this process, layer formation arises at the surface, ion exchange occurs as well as dissolution of the altered surface. These changes at the interface glass - corrosion media were first observed with in-situ microscopy. Corrosion tests were executed under static and dynamic test conditions, in order to gain information about the dependence on time, temperature and ratio of sample surface to solution volume. The developed layers were analysed after the corrosion tests with scanning electron microscopy with energy dispersive analysis in order to gain elemental concentration profiles. Raman microscopy and infrared reflexion spectroscopy were used for identification of water species and their amounts. Besides layer characterisation, the gained corrosion values (pH value, concentration of dissolved species in the solution) were compared with established corrosion models.

O 36.68 Tue 18:15 Poster B2

Adsorption of tetrahydrofuran on the Si(001) surface studied by means of STM and XPS — •Marcel Reutzel[1], Gerson Mette[1], Michael Dürr[1,2], Ruben Bartholomäus[3], Ulrich Koert[3], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — [2]Fakultät Angewandte Naturwissenschaften, Hochschule Esslingen, D-73728 Esslingen — [3]Fachbereich Chemie, Philipps-Universität, D-35032 Marburg

A promising possibility to compete with the challenges of miniaturization in semiconductor device physics is the functionalization of inorganic semiconductor surfaces with organic molecules. In this context, we have investigated the reaction of the frequently-used organic solvent tetrahydrofuran (THF) on Si(001) by means of scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). Despite its low reactivity in solvent based organic chemistry, THF was found to exhibit a complex surface chemistry on the Si(001) surface.

At low temperatures, the STM images indicate an adsorption geometry with the THF molecule located at the lower Si dimer atom. In combination with an observed energetic shift to higher binding energies in the O(1s) XP spectra, a dative bonding between a free electron pair of the oxygen atom and the empty dangling bond surface state is suggested. At temperatures $T_s > 270$ K, an irreversible rearrangement of the THF molecules is observed. The resulting configurations bridge two dimer rows. For temperatures $T_s > 700$ K, the STM and XPS data point to the formation of silicon carbide and silicon oxide structures.

O 36.69 Tue 18:15 Poster B2

CH_4 and C_2H_4 decomposition and hydrocarbon formation on Ru(0001) — •Harald Kirsch, R. Kramer Campen, and Martin Wolf — Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin

Interaction of CH_4 and C_2H_4 with a metal (oxide) surface may lead to the stepwise decomposition of these species and the formation of higher hydrocarbons. Understanding the details of these processes is critical to engineer desired chemistry: e.g. the oxidative coupling of CH_4 to form C_xH_y or the steam reforming of CH_4. Here we characterize the interaction of CH_4 and C_2H_4 with the Ru(0001) surface under UHV conditions using temperature programmed desorption and vibrational sum frequency spectroscopy (> 5 cm^{-1} resolution) as a function of surface temperature (100-500 K) and coverage (quantified using C+O recombinative desorption). To overcome the dissociation barrier of CH_4 on Ru(0001) we employ a molecular beam source with CH_4 seeded either in He or H_2. By investigating both CH_4 and C_2H_4 decomposition we identify novel species in the decomposition pathways of both gases: CCH_2 is observed in the sequential decomposition of C_2H_4 and CCH in the high temperature decomposition($> 350K$) of CH_4 each for the first time. By characterizing both species as a function of surface coverage and, for CH_4, as a function of carrier gas we further show how the relative stability of various double-carbon species is a function of available hydrogen adsorption sites. At coverages $< 30\%$ of a ML of carbon, the formed CCH_2/CCH species are stable up to 350K, while at $> 60\%$ ML its stable up to 500K. The results are discussed in comparison to theoretical modelling of the decomposition process.

O 36.70 Tue 18:15 Poster B2

Sabatier based CO2-Methanation of flue gas in conventional power plants — •Michael Fleige, Klaus Müller, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik/Sensorik, Konrad-Wachsmann-Allee 17, Germany

Already discovered by Paul Sabatier in 1902 the Hydrogenation according to CO2 + 4H2 ->CH4 + 2H2O nowadays is discussed in the course of the 'Power-to-Gas' approach to utilize excess energy from renewable electricity generation in times of oversupply of electricity. We investigate the behavior of this process in a simulated flue gas atmosphere of conventional base load power plants, which could be used as constant sources of the reactant CO2. Therefore the influence of different flue gas compositions such as varying contents of nitrogen and residual oxygen are tested in a laboratory scale. The heterogeneous catalysis process is investigated with regard to conversion rates, yield and selectivity and long-term stability of the Ni-catalyst. Earlier results of stable operating conditions in a 1:1 mixture of nitrogen and reactants, which is a typical ratio for flue gas in conventional power plants, could be confirmed in a first step.

O 36.71 Tue 18:15 Poster B2

HR-EELS on powder samples — •Sebastian Frey, Martin Kroll, and Ulrich Köhler — Ruhr-Universität Bochum

High resolution electron energy loss spectroscopy is a useful tool in heterogeneous catalysis as it provides information about vibrational states of adsorbates. While HR-EELS on single crystals has found wide spread and nowadays serves as a sophisticated tool to obtain adsorbate information, most studies on oxide nanoparticles rely on infrared spectroscopy (FTIRS) as EELS requires a reflecting sample with high conductivity. In the field of heterogeneous catalysis this causes a material gap between idealized single crystalline model systems (analyzed with HR-EELS) on the one hand and real catalysts based on nanoparticles (studied with FTIRS) on the other hand.

Enabling HR-EEL Spectroscopy on nanoparticles opens up a new approach to get closer insight into the behavior of real oxide materials that are used in heterogeneous catalysis. We studied ZnO nanoparticles and their corresponding metal loads Cu and Au, which are used for methanol synthesis and CO oxidation. Our experience shows that a thoroughly sample preparation and pretreatment is vital in order to obtain reasonable results in the EELS. The nanoparticle layer has to be smooth and closed to produce adequate reflection intensity. Moreover sufficient conductivity is required to prevent surface charging. Both requirements can be met by sedimenting oxide powder on a gold plate. In the case of ZnO a clear phonon spectrum emerges which is comparable to Fuchs-Kliewer phonons present on a single crystalline surface.

O 36.72 Tue 18:15 Poster B2

Ultraviolet photoelectron spectroscopy and transmission electron microscopy of mass selected silver clusters — •Natalie Miroslawski[1], Christoph Schröder[1], Paul Salmen[1], Bernd von Issendorff[2], Wilfried Sigle[3], Peter A. van Aken[3], and Heinz Hövel[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Fakultät für Physik, Albert-Ludwigs Universität Freiburg, 79104 Freiburg, Germany — [3]MPI for Intelligent Systems, 70569 Stuttgart, Germany

Mass selected silver clusters between 55 and 923 atoms were deposited with less then 0.1eV/atom kinetic energy on Xenon and investigated with ultraviolet photoelectron spectroscopy (UPS) with a photon energy of 11.6eV. The clusters were deposited with different coverage and measured at 15K. To extract the signal of the silver clusters we measured spectra for the rare gas covered substrate before deposition and substracted them from the measurements after cluster deposition. We obtained a size dependent cluster signal for energies in the s-p-band region which are discussed in respect of free beam experiments [1].

Additionally we present transmission electron microscopy (TEM) images of silver clusters with 923, 1100 and 2493 atoms per cluster.

[1] Oleg Kostko, *Photoelectron spectroscopy of mass-selected sodium, coinage metal and divalent metal cluster anions*, PhD-thesis, Albert-Ludwigs-Universität Freiburg (2007)

O 36.73 Tue 18:15 Poster B2

Mass selected copper clusters on rare gases(Ar/Xe): Photoelectron spectroscopy with ultraviolet light — •Paul Salmen[1], Natalie Miroslawski[1], Christoph Schröder[1], Bernd von Issendorff[2], and Heinz Hövel[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Fakultät für Physik, Universität Freiburg, 79104 Freiburg, Germany

We investigated mass selected copper clusters between 55 and 923 atoms deposited and measured at temperatures between 12 K and 15 K on several monolayers of Argon (Ar) and Xenon (Xe) using ultraviolet photoelectron spectroscopy. The rare gas was used to minimize the cluster/surface interaction and the layers were adsorbed at 30 K (Xe) and 15 K (Ar) on Copper(111) and Silver(111) surfaces. The clusters were soft landed with less than 0.1 eV per atom kinetic energy. To extract the signal of the copper clusters we measured the spectra for the rare gas covered substrate before deposition and subtracted them from measurements after the deposition. We used an Ar-gas discharge lamp ($h\nu$=11.6 eV) with a heatable LiF-window to suppress the satellite lines[1].

[1] M.Budke and M.Donath, Appl. Phys. Lett. 92, 231918 (2008); S.Suga, et al., Rev. Sci. Instruments 81, 105111 (2010)

O 36.74 Tue 18:15 Poster B2

High deposition rate of metal (oxide) nanoclusters generated in pulsed DC magnetron sputtering system — •Oleksandr Polonskyi[1,2], Tilo Peter[1], Amir Ahadi[1], Alexander Hinz[1], Thomas Strunskus[1], Vladimir Zaporojtchenko[1,3], and Hynek Biederman[2] — [1]Faculty of Engineering, Institute for Materials Science - Multicomponent Materials, Kiel University, Kaiserstr. 2, D-24143 Kiel, Germany — [2]Charles University in Prague, Faculty of Mathematics and Physics, V Holesovickach 2, 180 00 Prague 8, Czech Republic — [3]deceased

The effect of pulsing a DC magnetron discharge on deposition of metal (-oxide) nanoclusters was studied. The work is focused mainly on the deposition of Ti (TiOx) nanoclusters by means of gas aggregation cluster source based on magnetron sputtering. Argon was used as a working gas and additionally, a low concentration of oxygen was admixed, which is necessary for the cluster formation process. The discharge was excited using the combination of a DC power supply operating at constant power mode and self-constructed pulsing unit with frequency repetition up to 100 kHz. It was found that the utilization of pulsed magnetron sputtering provides an extremely high deposition rate of Ti (TiOx) nanoclusters in comparison to a continuous magnetron discharge. The influence of the discharge repetition frequency (20-100 kHz) and duty cycle (20-90%) was investigated. By adjusting the duty cycle and repetition frequency at constant power and oxygen admixture, a maximum efficiency of cluster generation and thus deposition rate can be found.

O 36.75 Tue 18:15 Poster B2

Clusters from Focused Ion Beams – High-resolution mass spectroscopy of Liquid Metal Ion Sources — •Martin Wortmann, Dirk Reuter, and Andreas D. Wieck — Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum

The Liquid Metal Ion Source (LMIS) is by far the most commonly used source type for Focused Ion Beam (FIB) applications. But the expected abundance of clusters from these sources also makes them a promising tool for the preparation of mass selected clusters. For the investigation of the emission characteristics, the resolution of the FIB-system-built-in mass filters is normally the limiting factor. The resolution of the commonly employed $E \times B$ – filters decreases with the mass of the clusters and therefore it has so far been impossible to measure the abundance of clusters, which are composed of more than 10 atoms.

Recently, a high resolution mass spectrometer for measuring the emission characteristics of LMIS has been built and set into operation. The resolution of the measurement setup is sufficient for accomplishing mass separation for clusters with masses above 2000 amu. Small clusters can even be analyzed regarding their composition of different isotopes. In this contribution, technical details of the mass spectrometer and results of the first measurements are presented.

O 36.76 Tue 18:15 Poster B2

Structural and Dynamical Properties of Nitrates of Alkali Metal in the Vapor-aqueous Interface — •Gang Huang — Institute for Pysics, University of Mainz,Mainz, Germany

The structure of ions at the vapor-aqueous interface, and their influence on the water's hydrogen bond network is of special interest to the atmospheric chemistry community. The use of surface specific vibrational spectroscopy techniques has permitted to elucidate some aspects of surface hydrogen bond structure for water in the presence of ions [1]. The influence of molecular ions (such as nitrate and sulfate ions) has been analyzed, but proved more elusive than that for halide solution [2].

We use ab initio molecular dynamics to analyze the structure and dynamics of the vapor-aqueous interface containing LiNO3 and to provide a microscopic interpretation of recent experimental results from the group of H. Allen. Vibrational density of states is used to extract the vibrational signatures for the ions and the surrounding water molecules. Gas phase clusters of (Alkali)NO3(H2O)n (n=3,4,5) have been used to obtain the effects of different Alkali ions on hydrogen bond network. The MD simulations were performed with the software suite CP2K.

[1] A. Jubb, W. Hua, and H. Allen, Ann. Rev. Phys. Chem. 2012, 63:107

[2] S. Gopalakrishnan, P. Jungwirth, D. Tobias, and H. Allen, J. Phys. Chem. B 2005, 109, 8861-8872

O 36.77 Tue 18:15 Poster B2

Synthesis of core-shell and composite nanoparticles — •Aladin Ullrich, Stefan Hohenberger, and Siegfried Horn — Lehrstuhl für Experimentalphysik II, Universität Augsburg

We have investigated the synthesis of core-shell and composite transition metal oxide nanoparticles. The particles were synthesized by thermal decomposition of metallorganic precursors in a high-boiling solvent. We synthesized particles consisting of a mixture of iron oxide and manganese oxide in a two-step synthesis.

In the first step, iron oleate and manganese oleate were used as precursors for the production of pure iron oxide and manganese oxide nanoparticles, respectively. In the second step, these particles were used as seed crystals for the growth of the respective other compound. Following this route we were able to synthesize composite particles combining iron oxide and manganese oxide. The particles were characterized by transmission electron microscopy, using the energy filtered imaging mode to visualize the elemental distribution. The composite particles found included also core-shell-systems with a size of 20 nm.

The magnetic properties of the particles were studied on a sample produced by drying a solution of hexane containing composite particles. Field cooled magnetic hysteresis measurements show an exchange bias. We suggest that this exchange bias arises from the interface between manganese oxide and iron oxide within the composite particles.

The preparation method for composite nanoparticles described here is widely applicable, e.g. it can be applied to almost all transition metal oxides.

O 36.78 Tue 18:15 Poster B2

Interaction of Metal Clusters with Organic Molecules: Absorption Spectroscopy and Current Setup of a Photoemission Electron Microscope — •Hannes Hartmann[1], Ingo Barke[1], Vladimir Popok[2], Alexandra Pazidis[1], Antje Neubauer[1], Stephan Bartling[1], Stefan Lochbrunner[1], and Karl-Heinz Meiwes-Broer[1] — [1]Institut für Physik, Universität Rostock, Universitätsplatz 3, 18051 Rostock, Germany — [2]Department of Physics and Nanotechnology, Aalborg University, 9220 Aalborg, Denmark

Clusters and nanoparticles are of significant interest for applications in catalysis. One approach is the utilization of the nanoparticles' optical properties to increase the efficiency of existing catalytic schemes. In this contribution recent results on the optical properties of a system of Ir based photosensitizers (PS) in interaction with Ag clusters are summarized in view of potential applications for photocatalytic hydrogen production. For a more detailed understanding of the coupling mechanisms between deposited clusters and organic molecules an experimental setup for photoemission electron microscopy (PEEM) is being realized. The PEEM is equipped with an imaging time-of-flight and a retarding-field energy filter. Several excitation sources can be used, including a Hg-lamp, a 266nm cw-laser, and a Ti:sapphire laser for two-photon photoemission (2PPE). In addition to standard equipments for sample preparation the chamber is attached to a cluster source for in-situ deposition of mass-selected nanoparticles. The current state of design and construction of the experimental setup, as well as the results of first measurements are presented.

O 36.79 Tue 18:15 Poster B2

UV-VIS absorption and XANES of Ag clusters in matrices

— •Stefanie Duffe[1], David Engemann[1], Sabrina Hoffmann[1], Christian Sternemann[1], Ralph Wagner[2], Kristina Kvashnina[3], Pieter Glatzel[3], and Heinz Hövel[1] — [1]TU Dortmund, Fakultät Physik / DELTA, Dortmund, Germany — [2]BU Wuppertal, Fachgruppe Physik-Materialwissenschaften, Wuppertal, Germany — [3]ESRF, Grenoble, France

We produce Ag clusters by supersonic nozzle expansion using THECLA, a THErmal CLuster Apparatus [1,2] which was designed to enable optical spectroscopy of clusters in a free jet and deposited on silica glass [2] or in matrices. The optical properties and the UV-VIS absorption band of Ag clusters alter significantly with size, shape, interparticle spacing and the properties of the local environment. Embedding the clusters into polydimethylsiloxane (PDMS) [3], aerogel or ionic liquids enables the investigation of a much higher amount of separated clusters which is otherwise limited by coalescence and electromagnetic coupling. We investigate the plasmon resonance of Ag clusters in PDMS or aerogel by optical spectroscopy [4]. XANES measurements at the Ag $L_{1,2,3}$-edges [5] were carried out at the synchrotron radiation sources DELTA and ESRF and were compared to FEFF calculations.

[1] O. F. Hagena, Z. Phys. D 20, 425 (1991). [2] H. Hövel et al., Phys. Rev. B 48, 18178 (1993). [3] L. Ravagnan et al., J. Phys. D 42, 082005 (2009). [4] U. Kreibig et al. In: Advances in Metal and Semiconductor Clusters Vol. 4, (ed. M.A. Duncan), JAI press Inc., 345 (1998). [5] P. Behrens et al., Z. anorg. allg. Chem. 625, 111 (1999).

O 36.80 Tue 18:15 Poster B2

Conductance and Relaxations of Magnetic Single-Atom Contacts

— Nicolas Néel[1], Silke Schröder[2], Cesar Lazo[2], Paolo Ferriani[2], Nico Ruppelt[1], •Jörg Kröger[3], Stefan Heinze[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [3]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

Single-atom contacts fabricated from a Cr-covered tip of a scanning tunnelling microscope and Co and Cr atoms adsorbed to Fe double-layer islands on W(110) exhibit spin-dependent conductances. Depending on the alignment of the magnetic moments of the tip apex and the adsorbed atom the conductance varies by ≈ 40 %. Consequently, these contacts represent atom-sized spin valves. Scrutinizing the spin polarization of the current through these contacts in the vicinity of the tunneling-to-contact transition reveals different geometric relaxations depending on the magnetic moment alignment. Concomitant density functional calculations trace these observations to differently strong exchange forces. The tunnelling anisotropic magnetoresistance is explored at the ultimate limit, *i. e.*, at the single-atom scale. Single Co atoms adsorbed to domains and domain walls of a ferromagnetic Fe film on W(110) exhibit an anisotropy of the magnetoresistance of up to 12 % and repeated sign changes as a function of the bias voltage. Financial support by the Deutsche Forschungsgemeinschaft through SFB 668 is acknowledged.

O 36.81 Tue 18:15 Poster B2

Highly efficient spin-resolved photoelectron spectroscopy experiment

— •Moritz Plötzing, Roman Adam, Lukasz Plucinski, and Claus M. Schneider — Peter Grünberg Institut (PGI-6), Research Center Jülich, 52425 Jülich, Germany

The presented work aims for building up an energy- and spin-filtered photoemission setup enabling electron count rates high enough for pump-probe experiments using pulsed extreme ultraviolet light sources. In order to reach the needed efficiency, the experiment is equipped with a high-transmission spectrometer as well as a spin-detector based on photoelectron scattering from a thin, oxidized iron film. The latter has a figure of merit $FOM = S^2 I/I_0$ (1) of 2.2×10^{-3} for a measurement of both orthogonal spin directions beeing more than one order of magnitude higher compared to other commercially available spin-detectors [1]. First results using a He discharge lamp on thin Co films in-situ grown on Cu(100) verify the high scattering efficiency $I/I_0 \approx 10\%$ in spin-resolved operation mode. Additionally, the determined spin-polarization $P \approx 30\%$ in the electrons below valence band is comparable with other published data and hence confirms the expected Sherman function, too. Both together serves as a proof of the high FOM.

(1): S: Sherman function, I/I_0: spin-resolved count rate normalized to count rate for incoming electrons

[1] M. Escher et al., *FERRUM: A New Highly Efficient Spin Detector for Electron Spectroscopy*, e-J. Surf. Sci. Nanotech. Vol. 9 (2011)

O 36.82 Tue 18:15 Poster B2

Complex magnetism in the Fe monolayer on Ir(001)

— •Markus Hoffmann, Maren Kaluza, Tobias Dornheim, Bertrand Dupé, Paolo Ferriani, and Stefan Heinze — Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel

Recently, complex magnetic ground states have been reported for a number of transition-metal nanostructures on surfaces [1-4]. The driving force behind these non-collinear spin structures is a competition of exchange, Dzyaloshinskii-Moriya (DM) and higher-order spin interactions. For an Fe monolayer on Ir(111) this leads to the formation of an atomic-scale magnetic skyrmion lattice [4]. Here, we present a first-principles study of the magnetic properties of the Fe monolayer on Ir(001) based on density-functional theory using the full-potential linearized augmented plane wave (FLAPW) method. We map our total energy calculations of spin spirals to a Heisenberg model to obtain the exchange constants. By including spin-orbit coupling we also find the strength of the DM interaction and the magnetocrystalline anisotropy. We demonstrate that higher-order spin interactions are non-negligible in this system. Based on the obtained magnetic interactions, we perform Monte-Carlo simulations and simulate spin-polarized scanning tunneling microscopy images.

[1] P. Ferriani *et al.*, Physical Review Letters **101**, 027201 (2008)
[2] Y. Yoshida *et al.*, Physical Review B **85**, 155406 (2012)
[3] M. Menzel *et al.*, Physical Review Letters **108**, 197204 (2012)
[4] S. Heinze *et al.*, Nature Physics **7**, 713 (2011)

O 36.83 Tue 18:15 Poster B2

Nanomagnets affected by spin-polarized tunneling and field-emission

— •Johannes Friedlein, Anika Schlenhoff, Stefan Krause, Andreas Sonntag, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

Understanding the interaction of spin-polarized electrons with magnetic solids is a key aspect in advanced spin-electronic applications. In general, a spin-polarized current affects a nanomagnet by Joule heating and magnon generation. In order to investigate similarities and differences of the interaction of tunneling and field-emitted electrons with magnetic matter on the atomic scale, we performed a combined spin-polarized tunneling microscopy (SP-STM) and spin-polarized scanning field-emission microscopy (SP-SFEM) study [1,2]. From a detailed lifetime analysis of a thermally switching nanomagnet, we extract the impact of spin-polarized tunneling and field-emitted electrons on Joule heating and spin-transfer torque. Whereas tunneling electrons carry low-energy into the magnet, high-energy field-emitted electrons are injected into the spin-dependent image potential states located in the vacuum in front of the magnet and subsequently relax into the sample [3]. We will present the experimental results in terms of current-dependent generation of Joule heating, magnons and Stoner excitations.

[1] S. Krause *et al.*, Phys. Rev. Lett. **107**, 186601 (2011).
[2] A. Schlenhoff *et al.*, Phys. Rev. Lett. **109**, 097602 (2012).
[3] A. Kubetzka *et al.*, Appl. Phys. Lett. **91**, 012508 (2007).

O 36.84 Tue 18:15 Poster B2

High-Frequency Vibrational Modes of Cold-Deposited Copper Adatoms on Low-Index Copper Surfaces

— •Jan Pischel, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

Vicinal low-index metal surfaces are known to give rise to vibrational modes with frequencies well above the bulk phonon band [1,2]. Low-coordinated atoms at steps and kink sites which relax with respect to their bulk position, but also with respect to their regular surface position, have been identified as originators of these high-frequency modes [2]. If the surface, the steps and the kinks are thought of as "perturbations of increasing complexity on an otherwise periodic system" [2], the next step would consequently be to investigate the vibrational properties of single adatoms.

For that purpose, we prepared copper surfaces with a well-defined degree of roughness under UHV by cold-depositing small amounts of copper on sputter-annealed low-index surfaces. Our HREEL-spectra of the rough Cu(111) and Cu(110) surfaces show indeed excitations at frequencies even higher than those observed on the vicinal surfaces. Since vibrations are playing a crucial role in the mediation of surface reactions [3], the existence of high-frequency vibrational modes on rough metal surfaces is expected to be relevant for a better understanding of catalytic reactions.

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[2] A. Kara et al., Phys. Rev. B **61**:5714–5718, 2000.

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O 36.85 Tue 18:15 Poster B2

Optimized Extreme-Ultraviolet High-Harmonic Generation Output for trARPES from Correlated-Electron Materials — •J. Urbancic[1], S. Eich[1], M. Wiesenmayer[1], A. V. Carr[2], A. Ruffing[1], S. Jakobs[1], S. Hellman[3], K. Jansen[3], A. Stange[3], M. M. Murnane[2], H. C. Kapteyn[2], L. Kipp[3], K. Rossnagel[3], M. Bauer[3], S. Mathias[1], and M. Aeschlimann[1] — [1]TU Kaiserslautern and Research Center OPTIMAS, 67663 Kaiserslautern, Germany — [2]JILA, University of Colorado and NIST, Boulder, Colorado 80309-0440, USA — [3]IEAP, University of Kiel, 24098 Kiel, Germany

Time- and angle-resolved photoemission spectroscopy (trARPES) using femtosecond laser pulses in the extreme ultraviolet (XUV) region plays a key role in the investigation of ultrafast quasiparticle dynamics in correlated-electron materials [1-4]. However, the full potential of this technique has not been achieved, i.e. all so far developed technical solutions suffered from a trade-off between photon flux, energy- and time-resolution. This was because of limitations in the intrinsic high-harmonic generation (HHG) process, and because of dispersive optical elements in the XUV-beamline that were needed to monochromatize the output of the HHG source. Here we show that using short-wavelength laser light to drive the HHG process and removing most of the dispersive elements offers an improved solution for efficient XUV trARPES with sub 30 fs time- and sub 150 meV energy-resolution.

[1] Rohwer et al., Nature 471, 490 (2011), [2] Petersen et al., PRL 107, 177402 (2011), [3] Carley et al., PRL 109, 057301 (2012), [4] Hellmann et al., Nat. Comm. 3, 1069 (2012)

O 36.86 Tue 18:15 Poster B2

Thermal desorption spectroscopy of astrophysically relevant molecules on olivine and single crystal forsterite — •Tushar Suhasaria[1,2], Nadine Heming[1], Robert Frigge[1], Björn Siemer[1], and Helmut Zacharias[1,2] — [1]Physikalisches Institut, University of Münster, Germany — [2]Graduate School of Chemistry, University of Münster, Germany

Over the years, it has been known that gas-grain chemistry is responsible for molecule formation in the interstellar medium [1]. These dust grains are thought to be silicates or carbonaceous materials. In recent times more than 140 different gases have been reported in the dense regions of interstellar space [2]. At low temperatures ($\approx$ 10 K) in the ISM the icy grain mantles undergo processing and are forming molecules due to exposure to ultraviolet, x-ray, cosmic radiation and heat. Temperature programmed desorption (TPD) is the most widely used characterization technique to investigate these primary effects and provide binding energies and reaction orders .Starting at 4K we performed TPD measurements on several molecules like D_2, CO, CH_4,CO_2 and NH_3 adsorbed on single crystal forsterite ($MgSiO_4$) and olivine (Mg_x Fe_{1-x} SiO_4) surfaces. Averaging over several measurements, it is seen that D_2, CO, CH_4, CO_2 molecules have slightly greater average binding energies on forsterite than on olivine.

1] D. A. Williams, E. Herbst, Surf. Sci. 500, 823, (2002).

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O 36.87 Tue 18:15 Poster B2

Probing shallow trapped electron state and related processes of TiO_2 with UHV-IRRAS — Hikmet Sezen, •Carsten Natzeck, Chengwu Yang, Alexei Nefedov, and Christof Wöll — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

TiO_2 as a metal oxide material with a wide band gap has numerous attentions because of its distinct chemical and physical properties. The shallow trapped electron state of TiO_2 presenting ca. 0.12 eV below than the conduction band continuum has not been fully understood property that has a crucial rule about photo- and charge-induced catalytic reactions.[1,2] In this work, a novel system for infrared reflection absorption spectroscopy in ultrahigh vacuum ambience (UHV-IRRAS) was used that allows recording both UHV-IRRAS measurements at grazing incidence on single crystal and FTIR transmission measurements for polycrystalline powder samples. It has been shown, that with this system can probe directly population of presenting charges within band gap of TiO_2. Comparative studies of the shallow trapped related processes were performed under atomic hydrogen treatment and exciting stimuli are exposing UV light. Moreover, as well as the steady state, the rapid scan measurements have been done to follow dynamic of the related processes.

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O 36.88 Tue 18:15 Poster B2

Details in the short-time response of the photo-induced CDW phase transition of 1T-$TiSe_2$ measured with femtosecond XUV photoemission — •S. Eich[1], J. Urbancic[1], M. Wiesenmayer[1], A.V. Carr[2], A. Ruffing[1], S. Jakobs[1], S. Hellmann[3], T. Rohwer[3], M.M. Murnane[2], H.C. Kapteyn[2], L. Kipp[3], K. Rossnagel[3], M. Bauer[3], S. Mathias[1], and M. Aeschlimann[1] — [1]TU Kaiserslautern and Research Center OPTIMAS, 67663 Kaiserslautern, Germany — [2]JILA, University of Colorado and NIST, Boulder, Colorado 80309-0440, USA — [3]Institute of Experimantal and Applied Physics, University of Kiel, 24098 Kiel, Germany

We use time- and angle-resolved photoemission spectroscopy (trARPES) with sub 150 meV energy and sub 30 fs time-resolution to study the photo-induced phase transition in the charge-density wave compound 1T-$TiSe_2$ [1]. The improved energy-resolution in comparison to our previous studies does now allow us to disentangle more details in the short-time response of this charge-density wave compound to an ultrafast laser excitation.

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

O 36.89 Tue 18:15 Poster B2

Time-resolved desorption of Hydrogen isotopes from HOPG by femtosecond laser pulses — •Robert Frigge and Helmut Zacharias — Physikalisches Institut, Universität Münster, Germany

The desorption of atomic hydrogen isotopes from HOPG is examined after surface excitation with fs-laser pulses at $\lambda = 400\,\mathrm{nm}$. Desorbed neutral H atoms are ionized using (2+1) REMPI via the 2s ← 1s transition, and are detected with a time-of-flight mass spectrometer. Velocity distribution measurements result in three maxima for fast, medium and very slow desorbed hydrogen atoms. By electron scattering calculations [1] of the vibrational excitation of the H-C bond the three maxima can be identified with different adsorption potentials, depending upon the neighboring H atom position on the graphene lattice. A nonlinear fluence dependence of the desorption yield allows two pulse-correlation experiments. As a result we derive a pulse-delay dependent yield with a FWHM of between 700 fs for the fast and about 1 ps for the slow desorbing atoms . These correlation times indicate short lifetimes of the excited electrons and support a calculation in the DIMET model.

[1]R. Frigge et al., Phy. Rev. Lett., **104**, 256102 (2010)

O 37: Invited Talk (Paul M. Koenraad)

Time: Wednesday 9:30–10:15 Location: H36

Invited Talk O 37.1 Wed 9:30 H36

Single impurities in semiconductors studied by STM — •Paul Koenraad — Eindhoven University of Technology

Single impurities play an increasingly important role in devices and fundamental physics. In the emerging field of solotronics, where a solitary dopant determines the optoelectronic functionality, many exciting successes have recently been obtained. We use a Scanning Tunneling Microscope (STM) to examine and manipulate single (magnetic) impurities close to a natural cleavage plane of the semiconductor host to unravel their properties that can be strongly affected by the semiconductor-vacuum interface.

Cross-sectional Scanning Tunneling Microscopy (X-STM) is a unique tool that allows controlling the ionization state of single impurities and spatially resolving the shape of the wavefunction of a single hole or electron bound to an impurity atom. Such information is very valuable for the identification of the character of the electronic state and its interaction with the environment which can be strained or involve optical and magnetic fields.

In this presentation I will discuss 1) wavefunction imaging of single impurities with a different chemical nature 2) Fe doped GaAs where we have shown that we can manipulate the oxidation or valence state of a single Fe impurity by controlling the population of an internal d-shell. 3) the behavior of single magnetic impurities in a strong magnetic field 4) a memory that is based on a single bistable Si impurity in the surface layer of GaAs. Optical and voltage dependent measurements in our STM revealed interesting properties of this bistable Si atom.

O 38: Topological Insulators (jointly with HL, MA, TT)

Time: Wednesday 9:15–13:00 Location: H16

O 38.1 Wed 9:15 H16

Topological Excitonic Superfluids in Three Dimensions — •Ewelina M. Hankiewicz[1], Youngseok Kim[2], and Matthew Gilbert[2] — [1]Wuerzburg University — [2]University of Illinois, Urbana

We study the equilibrium and non-equilibrium properties of topological dipolar intersurface exciton condensates within time-reversal invariant topological insulators in three spatial dimensions without a magnetic field. We elucidate that, in order to correctly identify the proper pairing symmetry within the condensate order parameter, the full three-dimensional Hamiltonian must be considered. As a corollary, we demonstrate that only particles with similar chirality play a significant role in condensate formation. Furthermore, we find that the intersurface exciton condensation is not suppressed by the interconnection of surfaces in three-dimensional topological insulators as the intersurface polarizability vanishes in the condensed phase. This eliminates the surface current flow leaving only intersurface current flow through the bulk. We conclude by illustrating how the excitonic superfluidity may be identified through an examination of the terminal currents above and below the condensate critical current. Reference: Phys. Rev. B 86, 184504 (2012).

O 38.2 Wed 9:30 H16

Bi_2Te_3: A dual topological insulator — •Tomáš Rauch[1], Markus Flieger[1], Arthur Ernst[2], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The class of $\mathcal{Z}_2$ topological insulators requires time reversal symmetry, while topological crystalline insulators require a mirror symmetry (an example is SnTe [1]).

We show that the well-known $\mathcal{Z}_2$ topological insulator Bi_2Te_3 with $\mathcal{Z}_2$ invariant $(1; 0\,0\,0)$ is also a topological crystalline insulator with mirror Chern number -1. This dual topological character allows to dope Bi_2Te_3 magnetically, thereby breaking time-reversal symmetry, while keeping the topological crystalline character. As a consequence, magnetized Bi_2Te_3 shows a Dirac state at its (111) surface shifted off the time-reversal invariant momentum $\overline{\Gamma}$, provided the magnetization is perpendicular to a mirror plane.

These fundamental features are elaborated by means of tight-binding calculations of both the bulk and the surface electronic structure as well as of the topological invariants. $\vec{k} \cdot \vec{p}$ model calculations and *ab initio* KKR calculations complement and support these results.

Our findings open a new path toward device applications that rely on topological insulators with magnetically controllable topological character.

[1] L. Fu, Phys. Rev. Lett. **106** (2011) 106802; T. Hsieh *et alii*, Nature Comms. **3** (2012) 982.

O 38.3 Wed 9:45 H16

Three-dimensional Models of Topological Insulator Films: Dirac Cone Engineering and Spin Texture Robustness — David Soriano[1], •Frank Ortmann[1], and Stephan Roche[1,2] — [1]Catalan Institute of Nanotechnology, Barcelona (Spain) — [2]ICREA, Barcelona (Spain)

Topological insulators feature surface states which exhibit certain robustness to disorder and which can be gapped due to inter-surface tunneling. By designing three-dimensional models of topological insulator thin films, we demonstrate a tunability of surface states and the odd number of Dirac cones on opposite surfaces by modifications of the atomic-scale geometry at the boundaries. [1,2] This enables the creation of a single Dirac cone at the Γ point as well as possible suppression of quantum tunneling between Dirac states at opposite surfaces. We further analyze the robustness of the spin texture to bulk disorder which may help in quantifying bulk disorder in materials with ultraclean surfaces. [2]

[1] L. Fu, C.L. Kane, and E.J. Mele, Phys. Rev. Lett. 98, 106803 (2007)

[2] D. Soriano, F. Ortmann, and S. Roche, Phys. Rev. Lett. (in press)

O 38.4 Wed 10:00 H16

Transport properties of point contacts between helical edge states — •Christoph P. Orth and Thomas L. Schmidt — University of Basel, Switzerland

We study a 2D topological insulator with helical edges that are connected by local electron tunneling. The edges are in contact with four reservoirs held at different chemical potentials. In contrast to existing theories, we treat the tunneling exactly but apply perturbation theory for the electron-electron interactions to calculate the current. Furthermore, we allow for a slow momentum dependent spin-rotation of the helical fields which can be created, e.g., by Rashba spin-orbit coupling. This allows inelastic spin-flip tunneling processes between the edges. Our results help to understand the interplay between electron-electron and spin-orbit interactions in topological insulators.

O 38.5 Wed 10:15 H16

Exotic magnetic properties of diluted magnetic binary chalcogenides — •Maia G. Vergniory[1], Xabier Zubizarreta[1], Mikhail M. Otrokov[2], Igor V. Maznichenko[3], Juergen Henk[3], Evgueni V. Chulkov[4], and Arthur Ernst[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Tomsk State University, Tomsk, Russia — [3]Martin-Luther-University, Halle-Wittenberg, Germany — [4]Donostia International Physics Center, Donostia-San Sebastian, Spain

Using first-principles Green function approach we studied electronic and magnetic properties of diluted magnetic binary chalcogenides A_2B_3, doped with transition metals substituing the A element. The electronic structure of the impurities in the chalcogenides is mainly featured by the crystal field splitting. We found that two main mechanisms are responsible for long-range magnetic order in these materials: hole mediated magnetism within the layer of A atoms and indirect interaction between magnetic moments via a B atom. We also estimated Curie temperature of these systems, which was found in good agreement with the available experimental data. Our results shed light on the understanding of magnetic interaction and control in toplogical insulators.

O 38.6 Wed 10:30 H16

Quasiparticle study of the bulk topological insulators Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 including spin-orbit coupling. — •Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present *GW* calculations of the topological insulators Bi_2Se_3 and Bi_2Te_3 within the all-electron FLAPW formalism and compare them with previous calculations. We extend the study to the topological insulator Sb_2Te_3, which poses additional problems when studied with *GW* based on non-relativistic density functional theory (DFT) as it exhibits a negative DFT band gap. In contrast to the previous *GW* calculations, we fully take into account spin-orbit coupling (SOC) allowing spin-off-diagonal elements in the Green function and the self-energy, and we discuss the differences to a simpler perturbative approach (*i.e.*, treating SOC on DFT level *a posteriori*). Additionally, we show that the inclusion of SOC induces fundamental changes in the Green function G, whereas changes in the screened interaction W are negligible. We also discuss the influence of off-diagonal elements of the self-energy matrix.

After inclusion of quasiparticle effects, we observe a direct band gap at the Γ point for Bi_2Se_3, in disagreement with predictions from DFT but in accordance with experiment. For all compounds, in the most critical case of the band-inversion region around the Γ point, we show that the *GW* effective masses are significantly different from DFT ones.

Funding was provided by the Alexander von Humboldt Foundation.

O 38.7 Wed 10:45 H16

Controllable magnetic doping of the surface state of a topological insulator — •A. Eich[1], T. Schlenk[1], M. Bianchi[2], M. Koleini[3], O. Pietzsch[1], T.O. Wehling[3], T. Frauenheim[3], A. Balatsky[4], J.-L. Mi[5], B. B. Iversen[5], J. Wiebe[1], A.A. Khajetoorians[1], Ph. Hofmann[2], and R. Wiesendanger[1] — [1]Institute for Applied Physics, Universität Hamburg, Germany — [2]iNano, Aarhus University, Denmark — [3]Bremen Center for Computational Materials Science, Universitiy of Bremen, Germany — [4]NORDITA, Stockholm, Sweden — [5]Center for Materials Crystallography, iNano, Aarhus University, Denmark

A combined experimental and theoretical study of doping individual Fe atoms into Bi_2Se_3 is presented. It is shown through a scanning tunneling microscopy study that single Fe atoms initially located at hollow sites on top of the surface (adatoms) can be incorporated into subsurface layers by thermally-activated diffusion. Angle-resolved photoemission spectroscopy in combination with ab-initio calculations within density functional theory suggest that the doping behavior changes from electron donation for the Fe adatom to neutral or electron acceptance for Fe incorporated into substitutional Bi sites. According to the calculations, these Fe substitutional impurities retain a large magnetic moment thus presenting an alternative scheme for magnetically doping the topological surface state. For both types of Fe doping, we see no indication of a gap at the Dirac point.

T. Schlenk et al., arXiv: 1211.2142v1 (2012) [cond-mat.mtrl-sci]
J. Honolka et al., PRL **108**, 256811 (2012)

Coffee break

O 38.8 Wed 11:15 H16

Induced superconductivity in the topological surface state of mercury telluride (HgTe) — •Luis Maier, Manuel Grimm, Peter Schüffelgen, Daniel Knott, Christopher Ames, Christoph Brüne, Philipp Leubner, Jeroen Oostinga, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, 97074 Würzburg

It has been recently demonstrated, that a strained grown layer of of HgTe is a 3D topological insulator (TI) exhibiting a single family of Dirac cone states at its surface. Since the bulk has nearly no carriers left, the transport through these structures is strongly dominated by the surface states [1].

Because of the prediction of creation of Majorana bound states [2] we are looking at a superconductor-TI interface. This talk presents our results on highly transparent S-TI-S junctions where we observe unusual behaviour in the Josephson current.

Preliminary results of this project are published in [3].

[1] C. Brüne et al., Phys. Rev. Lett. 106, 126803 (2011)
[2] L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008)
[3] L. Maier et al., Phys. Rev. Lett. 109, 186806 (2012)

O 38.9 Wed 11:30 H16

Strained bulk HgTe as a 3D topological insulator — •Cornelius Thienel, Christopher Ames, Philipp Leubner, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Universität Würzburg, Lehrstuhl für experimentelle Physik III

HgTe is a semimetal that has an inverted band structure. We show that strained on CdTe the HgTe opens a bandgap and becomes a 3D topological insulator (TI). By magnetotransport measurements we confirm the existence of a 2D topological state and observe QHE from the surface. An analysis of SdH oszillations allows us to distinguish between two TI surfaces perpendicular to the magnetic field that have different charge carrier densities due to different electrostatic environments. When structuring a top gate on the sample, we are able to match the carrier densities of the surface states and therefore see a sequence of odd integer Hall plateaus, as predicted by Dirac physics.

O 38.10 Wed 11:45 H16

Comparing scattering processes in topological insulators and giant Rashba semiconductors — •Peter Lemmens[1], Vladimir Gnezdilov[2], Dirk Wulferding[1], Patrik Recher[3], Helmuth Berger[4], Yoichi Ando[5], Angela Möller[6], R. Sankar[7], and Fang-Cheng Chou[7] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE, Kharkov, Ukraine — [3]IMAPH, TU-BS, Braunschweig — [4]EPFL, Lausanne, Switzerland — [5]ISIR, Osaka, Japan — [6]Dept. of Chemistry, Univ. Houston, USA — [7]CCMS, National Taiwan Univ., Taipei, Taiwan

Using Raman scattering experiments we probe scattering processes in BiTeI and topological insulators. In the former systems the surface termination, either by Iodine - Bi or Tellur - Bi determines the low energy scattering properties. A comparison of these surface induced signals with effects seen in topological insulators leads to a considerable gain of understanding of scattering mechanisms and the respective role of symmetry. Work supported by DFG, B-IGSM and NTH School for Contacts in Nanosystems.

O 38.11 Wed 12:00 H16

Local photocurrent generation in thin films of the topological insulator Bi_2Se_3 — •Christoph Kastl[1], Tong Guan[2], Xiaoyue He[2], Kehui Wu[2], Yongqing Li[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching, Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

We report on the optoelectronic properties of thin films of the three-dimensional topological insulator Bi_2Se_3 grown by molecular beam epitaxy. In spatially resolved scanning photocurrent experiments, we observe submicron photocurrent patterns with positive and negative amplitude [1]. The patterns are independent of the applied bias voltage, but they depend on the width of the circuits. We interpret the patterns to originate from a local photocurrent generation [2] due to potential fluctuations [3]. Furthermore, we verify and discuss the impact of the circular photogalvanic effect in optoelectronic Bi_2Se_3-based circuits [4].

[1] C. Kastl et al., arxiv: 1210.4743 (2012).
[2] J. C. W. Song and L. S. Levitov, arxiv:1112.5654 (2011).
[3] H. Beidenkopf et al., Nat. Phys. 7, 939 (2011).
[4] C. Kastl et al. (2013).

O 38.12 Wed 12:15 H16

$Bi_{1-x}Sb_x$(110): A non-closed packed surface of a topological insulator — Lucas Barreto, Wendell Simoes da Silva, Malthe Stensgaard, Søren Ulstrup, Marco Bianchi, •Xie-Gang Zhu, Matteo Michiardi, Maciej Dendzik, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center Århus University, 8000 Århus C, Denmark

Topological insulators are characterised by an insulating bulk band structure, but topological considerations require their surfaces to support gap-less, metallic states. Meanwhile, many examples of such materials have been predicted and found experimentally, but work has concentrated on the closed-packed (111) surface of the topological insulators. Thus, the theoretical picture of an insulating bulk embedded in a metallic surface from all sides of a crystal still needs to be confirmed. Here we present angle-resolved photoemission spectroscopy results from the (110) surface of the topological insulator $\mathrm{Bi}_{1-x}\mathrm{Sb}_x$ ($x \approx 0.15$). The observed band structure and Fermi contour is in excellent agreement with theoretical predictions and slightly different from the electronic structure of the parent surface Bi(110), in particular around the X_1 time-reversal invariant momentum. We argue that the preparation of surfaces different from (111) opens the possibility to tailor the detailed electronic structure and properties of the topological surface states.

O 38.13 Wed 12:30 H16

Charge screening at the surface of a topological insulator: Rb on $\mathbf{Bi_2Se_3}$ — •Peter Löptien, Lihui Zhou, Jens Wiebe, Alexander A. Khajetoorians, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Germany

Adsorption of Rb atoms on $\mathrm{Bi_2Se_3}$ leads to the formation of a two-dimensional electron gas (2DEG) in the conduction band at the surface of the topological insulator [1]. We investigated the coverage dependent distribution of the singly charged Rb atoms by low temperature STM. By a statistical analysis of the interatomic distances between the adatoms we quantitatively derived the pair interaction [2], which fits a screened Coulomb potential. Interestingly, screening length and dielectric constant turn out to be rather small, due to the contribution of the 2DEG and topological surface state.

[1] M. Bianchi, R. C. Hatch, Z. Li, P. Hofmann, F. Song, J. Mi, B. B. Iversen, Z. M. Abd El-Fattah, P. Löptien, L. Zhou, A. A. Khajetoorians, J. Wiebe, R. Wiesendanger, and J. W. Wells, ACS Nano 6, 7009 (2012)

[2] J. Trost, T. Zambelli, J. Wintterlin, and G. Ertl, Phys. Rev. B 54, 17 850 (1996)

O 38.14 Wed 12:45 H16

Fabrication and characterization of thin Bi_2Se_3 topological insulators — •Srujana Dusari[1], Philipp Meixner[1], Anna Mogilatenko[2], Saskia F. Fischer[1], Jaime Sanchez-Barriga[3], Lada V. Yashina[4], Florian Kronast[3], Sergio Valencia[3], Akin Ünal[3], and Oliver Rader[3] — [1]Novel Materials, Humboldt Universität zu Berlin, D-12489 Berlin — [2]Ferdinand Braun Institut, D-12489 Berlin — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, D-12489 Berlin — [4]Dep. Chemistry, Moscow State University, Russia

Topological insulators (TIs) have electrically insulating states in the bulk and robust conducting states along the edges [1, 2]. The real-life TI samples available today contain residual bulk charge carriers that hinder exploiting their surface properties in device form. The aim of our work is to investigate the controlled combination of dimensionality and designed impurity and metallic defect structures on the quantum transport properties of well known Bi_2Se_3 TIs, in particular with respect to the implications for devices. Here we report preparation and characterization of exfoliated Bi_2Se_3 flakes. The samples are characterized using atomic force microscopy, transmission electron microscopy, and energy-dispersive X-ray spectroscopy. Surface stability and composition are determined using photoemission electron microscopy. Low temperature transport measurements are presented.

[1] C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).

[2] M. Z. Hasan and J. E. Moore, Annu. Rev. Condens. Matter. Phys. 2: 55-78 (2011).

O 39: Graphene: Characterization and Devices (jointly with DS, HL, MA, and TT)

Time: Wednesday 9:30–13:00 Location: H17

O 39.1 Wed 9:30 H17

Polarization dependence of phonon modes in graphene nanoribbons — •Felix Kampmann[1], Nils Scheuschner[1], Bernat Terrés[2,3], Christoph Stampfer[2,3], and Janina Maultzsch[1] — [1]Institut für Festkörperphysik, TU Berlin, Hardenbergstraße 36, 10623 Berlin, Germany, EU — [2]JARA-FIT and II. Institute of Physics B, RWTH Aachen University, Aachen, Germany, EU — [3]Peter Grünberg Institute (PGI-6/8/9), Forschungszentrum Jülich, Jülich, Germany, EU

Polarization dependent Raman spectroscopy has lately been used to investigate the edge states of few layer graphene revealing insight into the selection rules of their Raman modes.

Here we report polarization dependent Raman measurements on single-layer graphene nanoribbons with varying width down to 30 nm.

We show that the $\cos^2(\theta)$ behavior of the intensity ratio I(D)/I(G) can be reproduced as it has already been known for the graphene edge states. Furthermore we found a similar behavior for I(D′)/I(G) and discuss the dependence on the nanoribbon width.

O 39.2 Wed 9:45 H17

Manifestation of charged and strained graphene layers in the Raman response of graphite intercalation compounds — Julio Chacon-Torres[1], •Ludger Wirtz[2], and Thomas Pichler[1] — [1]Faculty of Physics, University of Vienna, Austria — [2]Physics and Material Sciences Unit, University of Luxembourg, Luxembourg

We present recent Raman measurements together with a detailed analysis of potassium graphite intercalation compounds (GICs): stage II to stage VI (where stage n means one intercalant layer after every nth graphene layer). By ab-initio calculations of the charge densities and the electronic band dispersions, we demonstrate that most (but not all) of the charge donated by the K atoms remains on the outer graphene layers, i.e., the once adjacent to the intercalant layer. This leads to an electronic decoupling of the inner (uncharged) from the outer (charged) layers and consequently also to a decoupling of the corresponding Raman spectra: The G-line splits into two peaks and the 2D line is entirely due to the uncharged inner layers while the 2D line of the outer layers is suppressed due to the strong charging. The quantitative interpretation of the peak positions requires that the internal strain of the graphene layers is taken into account. This allows to unambiguously identify the Raman response of strained charged and uncharged graphene layers and to correlate it to the in-plane lattice constant. Raman spectroscopy is thus a very powerful tool to identify internal strain in single and few-layer graphene as well as to to identify the strain in nanoelectronic and optoelectronic devices or the local interfacial strain in other graphene composites.

O 39.3 Wed 10:00 H17

C–axis transport in graphite and few–layered–graphene — •Ole Pfoch, Yuri Koval, Michael Enzelberger, and Paul Müller — Department of Physics and Interdisciplinary Center for Molecular Materials, Universität Erlangen

Electrical transport in single or few layered graphene was intensively investigated during the last decade. However, most experiments were performed with electronic transport in the plane. Measurements in perpendicular direction are rare and the results are rather sensitive to materials properties. For instance, the literature data for the anisotropy of the electrical conductivity in plane and along the c–axis varies between 100 and 10 000. One of the reasons for the wide spread of anisotropy data might be a significant influence of structural defects. We reduce the influence of these defects by decreasing the cross section of the measured structures down to $2 \times 2\,\mu\mathrm{m}^2$. Mesa type structures were prepared by e–beam lithography and $\mathrm{O_2}$–plasma etching. The influence of the mesa size on the c–axis conductivity and its temperature dependence were investigated. We have found that the c–axis conductivity is rather sensitive to the prehistory of the sample and to the origin of the graphite material. We present our recent results and discuss the mechanism of c–axis electrical transport.

O 39.4 Wed 10:15 H17

Electronic transport of metallic thin films and islands on graphene with scanning tunneling spectroscopy — •Anne Holtsch, Hussein Shanak, Haibin Gao, and Uwe Hartmann — Institute for Experimental Physics, Saarland University, P.O. Box 151150, 66041 Saarbrücken

Electronic properties of graphene without and with metallic thin films and islands on top are investigated. The graphene layers are epitaxially grown on rhodium using a chemical vapor deposition (CVD) method. In a second step, metallic thin films and islands (Au) are deposited onto the surface of the graphene layer. Investigations are performed by using scanning tunneling spectroscopy (STS). An introduction to a method for an automated comparison and characterization of different spectroscopic curves is the focus of this presentation. This method will be used to clarify which impact the metallic thin films and islands have on the electronic properties of graphene. Therefore a comparison between the results obtained from graphene samples without and with metalic thin films and islands is presented.

O 39.5 Wed 10:30 H17

Fano-Profiles in HOPG and graphene flakes. — •Matthias Städter, Matthias Richter, and Dieter Schmeisser — Brandenburg University of Technology, Cottbus, Germany

We investigated the electronic structure of the valence and conduction band of HOPG by 2D resonant photoemission spectroscopy. Our aim is to understand the electronic structure of defects and inhomogeneities in graphene and related materials in more detail. From our measurements we find that the transition from the σ-band to the π^*-band at the M-point shows a characteristic Fano-Profile. A Fano-Profile occurs as the result of the interference of the band to band transition and a parallel transition to a discrete energy level within the band gap.The theory of Fano enables us to determine the energetic location of these discrete level. It is found to be several meV above the Fermi-Energy. Additional measurements on graphene flakes lead to similar results for the σ- to π^*-band transition and the location of the discrete energy state. With this we not only can determine the energetic states of defects but also get a better understanding of the origin of the Fano profile which is a particular detail of the resonant absorption process.

O 39.6 Wed 10:45 H17

Multiple Auger Decay at resonant photo-excitation In carbon thin films — •Matthias Richter, Matthias Städter, Ioanna Paloumpa, and Dieter Schmeisser — Brandenburg University of Technology Cottbus, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

We use resonant photoemission at the C1s edge to study the electronic structure of HOPG, graphene flakes and monolayer graphene. We find remarkable differences in the profile of the Auger decay channels, which we attribute to an additional multiple-Auger with a three-hole final state. A prerequisite for the appearance of this decay mechanism is the existence of localized excitonic states, which cause the appearance of the multiple Auger decay. Defects (pits, holes, steps and kinks) can act as localized excitonic states. We use those effects to identify the existence and the quantity of such defect states within the π^*-band regime in carbon thin films, because the intensity of the three-hole Auger decay is varying with the defect density of the carbon films. The defect-excitonic states can be either localized in the band-gap at the M-point or in case of surface defects like steps, kinks or pits even at the K-point by losing the pure sp^2 character of the films. We find that the appearance of the multiple Auger decay is different for multilayer and monolayer graphene. In particular the interaction of impurities leads to broadening of the C1s core levels. The three-hole Auger decay spectroscopy is a new method to detect such contaminations with a high sensitivity.

O 39.7 Wed 11:00 H17

Characterization of large-scale graphene CVD with far-infrared radiation — •Christian Cervetti[1], Boris Gorshunov[1,4,5], Elena Zhukova[1,4,5], Martin Dressel[1], Klaus Kern[2,3], Marko Burghard[2], and Lapo Bogani[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Max Planck Institut für Festkörperforschung — [3]Institute de Physique de la Matière Condensée, Ecole Polytechnique de Lausanne, Switzerland — [4]A.M.Prokhorov General Physics Institute, Russian Academy of Sciences, Russia — [5]Moscow Institute of Physics and Technology (State University), Russia

We use monochromatic terahertz (THz) spectrometer and standard Fourier-transform spectrometer to measure the conductance of large scale single layer graphene obtained by chemical vapor deposition. We demonstrate the extreme sensitivity of the THz conductance to copper particles produced on graphene during the transfer process, making THz spectroscopy a powerful tool for monitoring the removal of unwanted leftovers during the production of large scale graphene samples.

Coffee break

O 39.8 Wed 11:30 H17

Terahertz generation in freely suspended graphene — •Andreas Brenneis[1], Leonhard Prechtel[1], Helmut Karl[2], Dieter Schuh[3], Werner Wegscheider[4], Li Song[5], Pulickel Ajayan[6], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, TU München, Germany — [2]Institute of Physics, University of Augsburg, Germany — [3]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [4]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland — [5]University of Science and Technology of China — [6]Rice University, Houston, Texas, USA

We report on THz generation and picosecond photocurrents in freely suspended bilayers of graphene [1]. The graphene layers are connected to coplanar strip lines which serve as source and drain contacts. A pump laser pulse excites charge carrier in the graphene. The resulting charge carrier dynamics couple to the strip line circuit and propagate along the strip line. With a probe laser pulse focused onto an on-chip photo switch, the propagating signal is read out via a third contact with a picosecond time resolution. By varying the delay of the probe pulse relative to the pump pulse, the optoelectronic signal can be measured time-resolved. We discuss the generation of THz radiation, ultrafast displacement currents, and thermoelectric currents within the optically excited graphene. Financial support by the ERC-grant NanoREAL is acknowledged.

References: [1] L. Prechtel, L. Song, D. Schuh, P. Ajayan, W. Wegscheider, A.W. Holleitner, Nature Comm. 3, 646 (2012).

O 39.9 Wed 11:45 H17

Broadband THz detection with graphene flakes — •Martin Mittendorff[1,2], Stephan Winnerl[1], Josef Kamann[3], Jonathan Eroms[3], Harald Schneider[1], and Manfred Helm[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Universität Dresden, Germany — [3]Universität Regensburg, Germany

We demonstrate a broadband THz detector based on graphene flakes, which are produced by scotch-tape method on SiO_2/Si, combined with a logarithmic periodic antenna. The antenna is coupled to the graphene flake with an interdigitated comb-like structure in the center. The detectors were characterized at roomtemperature using the free-electron laser FELBE at the Helmholtz-Zentrum Dresden-Rossendorf. The responsivity is above 1 nA/W for wavelengths from $30\mu m$ to $220\mu m$. The rise time of the measured signals is below 100 ps and their length is in the range of 200 ps, while the pulse duration of the FEL pulses is around 20ps. The effect of the antenna coupling could be confirmed via polarization dependent measurements. Due to the spectral bandwidth combined with high temporal resolution and simple handling these detectors can be very useful for timing purposes of short laser pulses.

O 39.10 Wed 12:00 H17

Electrostatic force and Raman spectroscopy measurements on graphene replicating water layers on mica — •Vitalij Scenev, Philipp Lange, Nikolai Severin, and Jürgen P. Rabe — Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Deutschland

Recently it has been argued that graphenes exfoliated onto mica become hole-doped by the substrate and that the doping level can be blocked by molecular water interlayers confined during sample preparation [1]. We use Scanning Probe Microscopy (SPM), Electrostatic Force Microscopy (EFM) and Raman Spectroscopy to investigate both the structure and the electronic properties of graphene conforming to molecular water layers on the mica surface. The layers are fluid, since variation of ambient humidity allows to control in-situ the layer thicknesses in the range of a monolayer [2]. Our data imply that graphene is hole-doped by the water layers with the doping level increasing with the water layer thickness.

1. Shim, J., et al., Water-Gated Charge Doping of Graphene Induced by Mica Substrates. Nano letters, 2012. 12(2): p. 648-654.
2. Severin, N., et al., Reversible dewetting of a molecularly thin fluid water film in a soft graphene-mica slit pore. Nano letters, 2012. 12(2): p. 774-779.

O 39.11 Wed 12:15 H17

Tailoring the graphene/silicon carbide interface for monolithic wafer-scale electronics — •Stefan Hertel[1], Daniel Waldmann[1], Johannes Jobst[1], Andreas Albert[1], Matthäus Albrecht[1], Sergey Reshanov[2], Adolf Schöner[2], Michael Krieger[1], and Heiko B. Weber[1] — [1]Chair for Applied Physics, Erlangen, Germany — [2]ACREO AB, Kista, Sweden

The vision of graphene as future material for electronic devices is derived from impressive material parameters. However, it is evident that graphene will not readily take over the role of a semiconductor. In particular, an efficient switch is lacking due to graphene's missing bandgap.

By focusing not only on the graphene layer, but considering the silicon carbide (SiC) substrate as an essential part of the system, we developed an easy scheme to fabricate transistors with high ON/OFF ratio - suited for logic - by tailoring the interface between SiC and the graphene layer [1]. Therefore we currently work with two graphene materials on SiC: as grown monolayer graphene (MLG) and hydrogen intercalated quasi-freestanding bilayer graphene (QFBLG). We proved the high-quality ohmic contact of MLG to n-type SiC and also characterized the Schottky-like behavior of QFBLG.

Using these components we are currently able to demonstrate transistors with ON/OFF ratios exceeding 104 at room temperature in normally-on and normally-off operation mode. We present a concept for inverters using a resistor-transistor logic scheme.

[1] S. Hertel *et al.*, Nature Communications **3**, 957 (2012)

O 39.12 Wed 12:30 H17

Electrical interfacing of cells with graphene field effect transistors — •Felix Rolf, Lucas H. Hess, Tobias Schneider, Benno Blaschke, Moritz Hauf, and Jose A. Garrido — Walter Schottky Institut, TU München

The next generation of neuroprosthetic devices will need novel solid-state sensors with improved performance. Increased signal detection capability, better mechanical and physiological compatibility with living tissue, and in general a higher stability in biological environments are among the main requirements. Due to its electronic and electrochemical characteristics, as well as its physico-chemical properties, graphene is one of the most suitable candidates to meet these demanding requirements.

In this talk, we will report on arrays of graphene solution-gated field effect transistors (G-SGFETs) which are able to detect the electrical activity of electrogenic cells. It will be discussed how the combination of high carrier mobilities in graphene and the large interfacial capacitance at the graphene/electrolyte interface results in such high signal sensitivities. Thereby it is possible for instance, to show the generation and propagation of action potentials in cardiomyocyte-like HL-1 cell cultures. Another application is the single cell-transistor coupling using Human Embryonic Kidney (HEK293) cells. In the latter case the response of the G-SGFETs to electrical activity as well as the cell chemical activity will be discussed. Our results confirm that G-SGFETs are able to outperform state-of-the-art devices, suggesting that G-SGFETs can play an important role in future bioelectronic systems.

O 39.13 Wed 12:45 H17

Exploring the electronic performance of graphene FETs for bio-sensing — •Lucas Hess, Benno Blaschke, Max Seifert, and Jose Garrido — Walter Schottky Institut, TU München

For medical applications such as neuroprostheses and for fundamental research on neuronal communication, it is of utmost importance to develop a new generation of electronic devices which can effectively detect the electrical activity of nerve cells. The outstanding electronic and electrochemical performance of graphene hold great promise for bioelectronic applications. For instance, we have reported on arrays of CVD-grown graphene solution-gated FETs (SGFETs) for cell interfacing, demonstrating their ability to transduce with high resolution the electrical activity of individual electrogenic cells.

In this contribution, we will present a detailed discussion on the suitability of CVD-grown graphene SGFETs for in-electrolyte operation, together with a study of the effect of electrolyte composition on the device performance. The sensitivity of SGFETs is dominated by two characteristic parameters: transconductance and electronic noise, which will be analyzed in this talk by in-electrolyte Hall-effect experiments and low-frequency noise characterization. Finally, we will briefly report on the pH and ion sensitivity of graphene devices, highlighting the influence of the chosen substrate for the device fabrication, as well as the effect of surface contamination from the fabrication technology.

This work demonstrates the potential of graphene to outperform state-of-the-art Si-based devices for biosensor and bioelectronic applications.

O 40: Spin Effects in Molecules at Surfaces (jointly with DS, MA)

Time: Wednesday 9:30–12:15 Location: H23

O 40.1 Wed 9:30 H23

Weak Coupling Kondo Effect in a Purely Organic Molecule: Universal Temperature and Magnetic Field Dependence — •Markus Ternes[1], Steffen Kahle[1], Yung-hui Zhang[1], Tobias Herden[1], Uta Schlickum[1], Peter Wahl[1,2], and Klaus Kern[1,3] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]School of Physics and Astronomy, University of St. Andrews, North Haugh, St. Andrews, Scotland — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The Kondo effect is one of the most intriguing any-particle phenomenon in solid-state physics due to the simplicity of the underlying model: the scattering of itinerant electrons at a localized spin.[1] It has been intensely studied on the single atomic and molecular level by scanning tunneling spectroscopy (STS) in the last two decades; however a quantitative comparison with theoretical predictions remained challenging due to orbital degeneracies and a spin quantum number higher than $\frac{1}{2}$. Here, we present STS measurements on an purely organic radical coupled to the conduction electrons of a Au(111) surface. The observed zero bias anomaly is due to a spin $\frac{1}{2}$ Kondo screening in the weak coupling limit. We can describe the temperature and magnetic field dependence of the spectral features practically parameter free by perturbation theory allowing quantitative tests on more complex theoretical models.

[1] A. C. Hewson, 1997: The Kondo Problem to Heavy Fermions, Cambridge University Press

O 40.2 Wed 9:45 H23

Density Functional Investigation of a Phthalocyanine Based Spin Transfer Material — •Rico Friedrich[1], Susi Lindner[2], Torsten Hahn[1], Claudia Loose[1], Martin Knupfer[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Freiberg, Germany — [2]IFW Dresden, Dresden, Germany

Interfaces were found to be of outstanding importance for electronic and spin transfer purposes especially in molecular spintronics [1]. Recently it has been demonstrated that an organic interface purely made from metal phthalocyanines namely manganese phthalocyanine (MnPc) and perfluorinated cobalt phthalocyanine (F_{16}CoPc) exhibits a charge and spintransfer at the interface between both molecules [2]. In this talk we present a systematic theoretical investigation of the phthalocyanine based dimer MnPc$^{\delta+}$/F_{16}CoPc$^{\delta-}$ within density functional theory framework. For all considered stackings a charge transfer from MnPc to F_{16}CoPc is observed which outlines this behavior as an intrinsic property of the molecular pair. In addition a ferromagnetic coupling ($S = 2$) of the molecular magnetic moments within the dimer is always observed due to 90° superexchange and direct exchange contributions. The comparison of the calculated absorption spectra of the geometrical arrangements to the experimentally recorded electron energy-loss spectrum strongly indicates the β-geometry to be preferred over all others. Only for this geometry an experimentally observed excitation around 0.6 eV is reproduced by the calculation.

[1] S. Sanvito, Nature Physics **6**, 562, (2010).
[2] S. Lindner *et al.*, Phys. Rev. Lett. **109**, 027601, (2012).

O 40.3 Wed 10:00 H23

Superexchange-mediated ferromagnetic coupling in two-dimensional Ni-TCNQ networks on metal surfaces — •Sebastian Stepanow[1], Nasiba Abdurakhmanova[1], Tzu-Chun Tseng[1], Alexander Langner[1], Christopher Kley[1], Violetta Sessi[2], and Klaus Kern[1,3] — [1]MPI-FKF Stuttgart — [2]ESRF Grenoble — [3]EPFL Lausanne

We investigate the magnetic coupling of Ni centers embedded in two-dimensional metal-coordination networks self-assembled from 7,7,8,8-Tetracyanoquinodimethane (TCNQ) molecules on Ag(100) and Au(111) surfaces. X-ray magnetic circular dichroism (XMCD) measurements show that single Ni adatom impurities assume a spin-quenched configuration on both surfaces, while Ni atoms coordinating to TCNQ ligands recover their magnetic moment and exhibit ferromagnetic coupling. The valence state and the ferromagnetic coupling strength of the Ni coordination centers depend crucially on the underlying substrate due to the different charge state of the TCNQ ligands on the two surfaces. The results suggest a superexchange coupling mechanism via the TCNQ ligands.

O 40.4 Wed 10:15 H23

Interface magnetism of the phenalenyl based molecular dimer adsorbed on a ferromagnetic surface — •Nicolae Atodiresei, Vasile Caciuc, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Molecular based magnetic units represent a very exciting avenue in designing and building future data storage, sensing and computing multifunctional devices. The density functional theory (DFT) provides a framework that reliably describes the electronic properties of molecules adsorbed on magnetic surfaces which are an essential perquisite for the design an understanding of the functionality of hybrid organic molecular spintronic devices. We will present *ab initio* studies performed to understand the interaction of a phenalenyl (PLY) based molecular dimer with a ferromagnetic Co surface. Charge transfer and hybridization between the atomic p_z orbitals of the PLY with the $d-$orbitals of the Co atoms create new hybrid metal-organic interface states [1,2] that lead to a large interfacial magnetoresistance near room temperature as measured in experiments [3]. Furthermore, our studies demonstrate the decisive role played by the van der Waals interactions in correctly describing the interaction between aromatic PLY dimers and metallic surfaces.

[1] N. Atodiresei *et al.*, Phys. Rev. Lett. **105**, 066601 (2010).
[2] N. Atodiresei *et al.*, Phys. Rev. B **84**, 172402 (2011).
[3] K. V. Raman *et al.*, accepted for publication in Nature (2012).

O 40.5 Wed 10:30 H23

Magnetism and molecule-surface interaction in transition metal porphyrin molecules on Cu(001) — •H. C. Herper[1,2], S. Bhandary[2], M. Bernien[3], C. F. Hermanns[3], A. Krüger[3], E. Weschke[4], C. Czekelius[5], C. Weis[1], C. Antoniak[1], B. Krumme[1], J. Miguel[3], D. Bovenschen[1], B. Sanyal[2], W. Kuch[3], H. Wende[1], and O. Eriksson[2] — [1]Fakultät für Physik und CeNIDE, Universität Duisburg-Essen, Germany — [2]Department of Physics and Astronomy, Uppsala University, Sweden — [3]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [4]Helmholtz-Zentrum Berlin, Germany — [5]Institut für Chemie und Biochemie, Freie Universität Berlin, Germany

We present a combined theoretical and experimental study of Fe(Co) porphyrin molecules on (O)/Cu(001) surfaces. The interaction between nonmagnetic surfaces and molecules is weak, hence the anisotropy of the molecule can be studied together with the influence of ligands and hybridization effects with the surface. Magnetic and structural properties have been investigated within DFT and angle-dependent X-ray absorption spectroscopy at the Fe $L_{2,3}$ edge. The magnetic dipole term is calculated to allow for comparison between spin moments from experiment and theory. The angle dependence of the calculated effective moments is in good agreement with the experimental findings. An intermediate spin state is obtained independent from the presence of an oxygen layer on the surface, which affects the hybridization between surface and molecule. A high-spin state can be realized by adding Cl or O ligands, which cause a stretching of the metal center-N bond.

15 min. break

O 40.6 Wed 11:00 H23

Magnetic coupling of Cobaltocene on magnetic surfaces through a graphene layer — •Simone Marocchi[1,2], Paolo Ferriani[3], Stefan Heinze[3], Franca Manghi[1,2], and Valerio Bellini[2,4] — [1]University of Modena and Reggio Emilia, Modena, Italy — [2]CNR Istituto di Nanoscienze S3, Modena, Italy — [3]Institute of Theoretical Physics and Astrophysics, Kiel, Germany — [4]CNR Istituto di Struttura della Materia, Trieste, Italy

The ability to improve the current electronic devices appear to be increasingly connected with the development of the molecule-based electronics [1] and spintronics [2]. We have concentrated our study, employing state-of-the-art density functional theory calculations, on the structural and magnetic properties of the Cobaltocene ($CoCp_2$) adsorbed on graphene deposited on slab of Ni(111). This molecule has been chosen because of its electronic structure rather unique among the metallocenes [3]. In several article has been pointed also out that graphene on Nickel (111) has mainly two energetically favored adsorption modes, namely top-fcc and bridge-top [4]. We will show how the magnitude of the magnetic coupling is drastically influenced by the structural factors named above and may vary by tens of meV. We further show how this coupling could be tuned by the intercalation of a magnetic monolayer, e.g. Fe and Co, between graphene and the Ni subtrate, and discuss the role of the graphene layer.

[1] X. Y. Zhu, Surf. Sci. Rep. 56, 1 (2004). [2] S. Sanvito, Chem. Soc. Rev. 40, 3336 (2011). [3] Y. Li, et al., Phys. Rev. B 83, 195443 (2011). [4] W. Zhao, et al., J. Phys. Chem. Lett. 2, 759 (2011).

O 40.7 Wed 11:15 H23

Atomic-scale Inversion of Spin Polarisation above an Organic-Antiferromagnetic Interface — •Nuala Mai Caffrey, Paolo Ferriani, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, Christian-Albrechts-Universität zu Kiel

The emerging field of organic spintronics aims to combine the advantantages of molecular electronics such as device miniaturisation and fabrication ease with the massive potential for application inherent in spintronics. Potential devices use organic molecules to control and manipulate spin-polarised signals. Such molecules are generally contacted with non-organic materials. As such, it is vital to understand the magneto-organic interface. It has been previously found that even the simplest non-magnetic molecule is capable of inverting the spin polarisation emerging from the clean ferromagnetic surface. We consider here an antiferromagnetic surface: a monolayer of Mn on a W(110) substrate. We perform *ab-initio* calculations in order to investigate the interface between simple organic molecules, both magnetic and non-magnetic, and an antiferromagnetic surface. The molecules considered include benzene (C_6H_6), cyclooctatetraene (C_8H_8) and small transition metal - benzene complexes. Simulated spin-polarised scanning tunnelling micoscopy (SP-STM) images are presented. They show that the exact magnitude and sign of the spin polarisation in the vacuum above the molecule is strongly dependent on the bonding details at the interface and due to the antiferromagnetic surface it exhibits a strong intra-molecular spatial dependence.

O 40.8 Wed 11:30 H23

Spin Crossover in a Vacuum-Deposited Submonolayer of a Molecular Iron(II) Complex — •Matthias Bernien[1], Dennis Wiedemann[2], Christian F. Hermanns[1], Alex Krüger[1], Daniela Rolf[1], Wolfgang Kroener[3], Paul Müller[3], Andreas Grohmann[2], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [3]Department of Physics, Universität Erlangen-Nürnberg, Erwin-Rommel-Straße 1, 91058 Erlangen, Germany

Spin-state switching of transition-metal complexes (spin crossover) is sensitive to a variety of tiny perturbations. It is often found to be suppressed for molecules directly adsorbed on solid surfaces. We present X-ray absorption spectroscopy measurements of a submonolayer of $[Fe^{II}(NCS)_2L]$ (L: 1-{6-[1,1-di(pyridin-2-yl)ethyl]-pyridin-2-yl}-N,N-dimethylmethanamine) deposited on a highly oriented pyrolytic graphite substrate in ultrahigh vacuum. These molecules undergo a thermally induced, fully reversible, gradual spin crossover with a transition temperature of $T_{1/2} = 235(6)$ K and a transition width of $\Delta T_{80} = 115(8)$ K. Our results show that, by using a carbon-based substrate, the spin-crossover behavior can be preserved even for molecules that are in direct contact with a solid surface.

Financial support by the DFG (Sfb 658: Elementary Processes in Molecular Switches on Surfaces) is gratefully acknowledged.

O 40.9 Wed 11:45 H23

Single spin-crossover molecules triggered with a STM — •Manuel Gruber[1,2], Toshio Miyamachi[1], Martin Bowen[2], Samy Boukari[2], Eric Beaurepaire[2], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Germany — [2]IPCMS (UMR 7504 UdS-CNRS) and Labex NIE, Strasbourg, France

A nano-scale molecular switch can be used to store information in a single molecule. The conductance of the molecule changes when switched and can be electrically detected. Spin crossover (SCO) molecules consisting of organic ligands around a transition metal ion are known to be switchable between a high- and a low-spin state by external stimuli [1]. It is the ultimate aim to achieve combined spin and conduction switching functionality on the level of individual molecules.

Fe(1,10-phenanthroline)2(NCS)2 molecules, SCO complexes, were deposited on Cu(100) and CuN/Cu(100) surfaces and studied with a scanning tunneling microscope (STM) in ultra-high vacuum at 4K.

Both spin species coexist at low temperatures as deduced from spectroscopic STM data. While on bare Cu(100), the molecules cannot be switched between the two spin states, molecules on CuN can individually and reproducibly be switched between a high-spin, high-conduction state and a low-spin, low-conduction state. This difference is explained by the role of the CuN layer to decouple the molecules from the metallic surface [2].

[1] P. Gütlich et al., Chem. Soc. Rev. 29, 419 (2000). [2] T. Miyamachi et al., Nat. Commun. 3, 938 (2012).

O 40.10 Wed 12:00 H23

Beyond the Heisenberg model: Anisotropic exchange interaction between a Cu-tetraazaporphyrin monolayer and Fe3O4(100) — •Hans-Joachim Elmers[1], Julia Klanke[2], Eva Rentschler[2], Katerina Medjanik[1], Dmytro Kutnyakhov[1], Gerd Schönhense[1], Sergey A. Krasnikov[3], Igor V. Shvets[3], Stefan Schuppler[4], Peter Nagel[4], and Michael Merz[4] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, D-55128 Mainz, Germany — [2]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Germany — [3]Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN) — [4]Karlsruhe Institute of Technology, Institut für Festkörperphysik (IFP), D-76021 Karlsruhe, Germany

We investigated the Heisenberg exchange coupling between the single Cu spin of Cu-tetraazaporphyrin deposited on magnetite(100) and the ferromagnetic surface using x-ray magnetic circular dichroism (XMCD). In contrast to the common model we find an anisotropic exchange coupling depending on the orientation of the spin relative to the bonding direction. The exchange coupling is ferromagnetic for magnetization direction perpendicular to the surface and antiferromagnetic for in-plane magnetization direction. The anisotropy of the Heisenberg exchange coupling is attributed to an orbitally-dependent exchange Hamiltonian. We propose that the sign change results from the competition between ferromagnetic superexchange along Fe-N-Cu and antiferromagnetic superexchange along Fe-O-Cu with strength modified by the strong spin-orbit coupling. Funded by COMATT.

O 41: Focussed Session: Frontiers of Electronic Structure Theory IV (jointly with HL and TT)

Time: Wednesday 10:30–13:30 Location: H36

Topical Talk O 41.1 Wed 10:30 H36

Challenges in data-intensive computational materials design: methodology and infrastructure. — •Boris Kozinsky — Robert Bosch Research and Technology Center, Cambidge, MA, USA

First-principles high-throughput screening of novel materials requires simultaneously inexpensive and accurate predictive computations of key properties. The first and most difficult challenge is the selection of the appropriate descriptors that are relevant to the material performance, and formulating the computational strategy. We will present examples of the computational design process in the fields of materials screening in batteries, catalysis and ferroelectrics. In each case, the critical issue is the selection of practical methods and validation using available data and higher-level models.

The second challenge is the need to establish a materials* informatics infrastructure able to automatically prepare and execute calculations on large classes of materials, to monitor calculations, and to store, retrieve and analyze complex data. We accomplish this by integrating storage databases with grid-enabled computational workflow into a powerful flexible environment adaptable to diverse purposes. We will discuss the requirements and possible use cases of such infrastructure elements. Together with collaborators, we are developing and making available this open-source software platform named AIDA (*Automated Infrastructure and Database for Atomistic design*) to make computational design efforts faster, easier, and fully integrated with automatic data collection and community sharing.

O 41.2 Wed 11:00 H36

DFT+U(ω): A simplified approach for dynamical Hubbard corrections to DFT: — •David D. O'Regan and Nicola Marzari — Theory and Simulation of Materials, EPFL, Switzerland.

Numerous successful techniques have been developed to date, such as DFT+U, in which the screened Coulomb interactions, underestimated by approximate density functionals, are described more accurately via a mapping onto the Hubbard Hamiltonian. Charge screening is a dynamical process, generally, and so to fully realise the capability of such methods for improving optical and quasiparticle spectra, the Hubbard U describing these interactions must gain a frequency dependence.

We introduce a simple and inexpensive approach, named DFT+U(ω), and readily implementable within an existing DFT+U or constrained-DFT code, in which the dynamical U tensor appropriate to the rotationally-invariant DFT+U functional is computed and used to correct DFT or static DFT+U spectra perturbatively. The rotationally-invariant DFT+U(ω) self-energy interpolates between static DFT+U and GW. We recast the density-functional linear-response approach for the static U, where it is defined as an energy curvature, within the language of many-body perturbation theory. Here, its dynamical generalisation, and its relationship to methods such as constrained RPA, becomes readily apparent. A plasmon-pole type model is used for the inverse dielectric function, whereby low-energy parameters are computed using the appropriately renormalised density-functional linear-response, and high-energy parameters are inexpensively approximated via independent-particle RPA or ALDA.

O 41.3 Wed 11:15 H36

Effective onsite interactions for materials with strong non-local Coulomb interactions — •Malte Schüler[1], Alexander Lichtenstein[2], Mikhail I. Katsnelson[3], and Tim Wehling[1] — [1]Institut für Theoretische Physik, Universität Bremen, D-28359 Bremen, Germany — [2]1. Institut für Theoretische Physik I, Universität Hamburg, D-20355 Hamburg, Germany — [3]Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands

sp-Electron systems and low-dimensional materials often comprise strong local Coulomb interaction and non-local Coulomb interaction at the same time. Here we report on a method to map a generalized Hubbard model with non-local Coulomb interaction to an effective Hubbard model with strictly local Coulomb terms U^*. With the examples of graphene and silicene we show that the non-local Coulomb interaction can reduce the effective local interaction up to a factor of 2. The U^* model is defined by a variational principle with respect to the free energy. In this framework, obtaining the effective interaction requires non-local charge correlation functions for various parameters of the effective Hubbard model, which are calculated by the determinant quantum Monte Carlo method. The temperature dependence of the effective interaction is discussed.

O 41.4 Wed 11:30 H36

First-principles calculation of Hubbard U parameters for half-metallic ferromagnets — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Correlation effects play an important role in the electronic structure of half-metallic ferromagnets (HM-FMs). They give rise to non-quasiparticle states above (or below) the Fermi energy at high temperatures [1], which reduce the spin polarization and as a consequence the efficiency of the spintronics devices. Employing the constrained random-phase approximation (cRPA) [2] within the full-potential linearized augmented-plane-wave (FLAPW) method [3], we have calculated the strength of the effective Coulomb interaction (Hubbard U) between localized $3d$ electrons in a series of HM-FMs like zincblende MnAs, half- and full-Heusler alloys NiMnSb and Co_2MnSi, respectively. The obtained Hubbard U parameters lie between 2.5 and 4.5 eV, being smallest for MnAs (Mn-$3d$) and largest for Co_2MnSi (Co-$3d$). The small value of U in the former can be attributed to the efficient screening of the As p electrons. For HM full-Heusler compounds the obtained U values are comparable to the ones in elementary $3d$ tran-

sition metals, while for half-Heusler compounds the U is a bit smaller.
[1] M. I. Katsnelson *et al.*, Rev. Mod. Phys. **80**, 315 (2008).
[2] E. Şaşıoğlu *et al.*, Phys. Rev. B **83**, 121101(R) (2011).
[3] http://www.flapw.de

O 41.5 Wed 11:45 H36

Magnetic Spectroscopies with DFT + Hubbard (U,V) — •Emine Kucukbenli[1], Davide Ceresoli[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH) — [2]CNR-ISTM Institute of Molecular Science and Technology, Milan (IT)

Hubbard U corrections to exchange-correlation functionals, introduced to deal with correlated electrons, have been shown to greatly improve the accuracy of DFT calculations of transition-metals, thanks to their ability to restore piecewise linearity of energy as a function of occupations and thus correct self-interaction errors. In addition, U is not a fitting parameter but can be calculated ab initio, using linear-response (LR) formulations.

Nevertheless, transition-metal complexes that display both covalent and ionic character are poorly described by DFT+U. Recently, the addition of an intersite Hubbard V is suggested to restore the accuracy of DFT+U for these cases, while V can be obtained ab initio as well.

In this study we combine DFT+U+V with the gauge-invariant projector augmented wave (GIPAW) method, and calculate magnetic spectroscopic properties of systems with transition metals. We have been implementing this combination in Quantum ESPRESSO package, both for LR and the recently introduced converse approach, that uses a much simpler Berry-phase calculation of the orbital magnetization. We then examine the performance of U+V corrections in determining the structural properties and hyperfine interaction parameters of small transition-metal molecules and complex organometallic systems.

O 41.6 Wed 12:00 H36

The magnetization of periodic solids from time-dependent current-density-functional theory. — •Arjan Berger[1,4], Nathaniel Raimbault[1,2], Paul de Boeij[3], and Pina Romaniello[2,4] — [1]Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier, IRSAMC, CNRS, Toulouse, France — [2]Laboratoire de Physique Théorique, CNRS, Université Paul Sabatier, IRSAMC, Toulouse, France — [3]Scientific Computing and Modeling, Amsterdam, The Netherlands — [4]European Theoretical Spectroscopy Facility

The evaluation of the macroscopic 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. For example, in case of the macroscopic polarization one can express the contribution of the charge density accumulated at the surface in terms of the bulk current density through the continuity equation. Therefore one can work in the framework of time-dependent current-density functional theory to efficiently calculate the macroscopic polarization [1,2]. In this presentation we will study how also the magnetization can be described within this framework.

[1] F. Kootstra, P. L. de Boeij, and J. G. Snijders, J. Chem. Phys. 112, 6517 (2000).

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

O 41.7 Wed 12:15 H36

Structure, charge order, phonons and IR spectra of magnetite — •Charles Patterson — School of Physics, Trinity College Dublin, Dublin 2, Ireland.

The structure and charge order of magnetite (Fe_3O_4) below the Verwey transition have been contentious issues for over 70 years. An x-ray refinement for the full 112 atom, Cc space group crystal structure of magnetite was reported only recently [1]. Previous refinements were hampered by multiple domain twinning in samples, whereas the recent study was performed on a micron-sized sample with two domains. Here we report hybrid density functional theory (DFT) calculations for the crystal structure, charge order, vibrations and IR spectra of magnetite in the Cc (112 atom) and $P2/c$ (56 atom) unit cells. Charge order in the Cc structure is found to consist of Fe trimerons, both in experiment [1] and calculations.

[1] M. S. Senn, J. P. Wright and J. P. Attfield, Nature 481, 173 (2012).

O 41.8 Wed 12:30 H36

Crystalline and Magnetic Anisotropy of the 3*d* Transistion-Metal Oxides — •Andreas Schrön[1], Claudia Rödl[1,2], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau, France

The 3d transition-metal oxides (TMOs) are subject of debate since many decades due to their extraordinary properties, such as the formation of an antiferromagnetic ordering AFM2 below their Néel temperature. Many studies, both experimental and theoretical, focus only on MnO and NiO, where the crystalline anisotropy is solely driven by exchange striction along the unique symmetry axis in the [111] direction and where the magnetic anisotropy is explained in terms of magnetic dipole interactions. In the other TMOs, FeO and CoO, however, orbital magnetization and spin-orbit interaction play an additional, yet crucial role for both crystalline and magnetic anisotropy.

We present density-functional theory (DFT) studies including an on-site interaction U of the crystalline and magnetic anisotropy of the electronic systems with non-collinear spins. The influence of the (semi-)local description of exchange and correlation (XC) by means of the local density approximation (LDA) and generalized gradient approximation (GGA) on the orbital moments in FeO and CoO and the implications on the aforementioned properties is investigated. We discuss the quenching of the orbital magnetization due to the gradient corrections.

O 41.9 Wed 12:45 H36

Electronic Structure and Magnetic interactions in 5*d* Ir oxide compounds — •Vamshi Mohan Katukuri[1], Viktor Yushankhai[2], Radu Coldea[3], Liviu Hozoi[1], and Jeroen van den Brink[1] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr. 20 01069 Dresden, Germany — [2]Joint Institute for Nuclear Research, Joliot-Curie 6, 141980 Dubna, Russia — [3]Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom

We investigate the correlated d-level electronic structure and magnetic interactions of 5d Ir oxide compounds by fully *ab initio* quantum-chemical many-body calculations on finite embedded clusters. The wave-function quantum-chemical methods provide a promising alternative to density-functional-based approaches to the electronic structure of solids. The computed d-d excitations in square-lattice, honeycomb, pyrochlore, and chain-like iridates compare well with recent RIXS (resonant inelastic x-ray scattering) data. We also perform a detailed analysis of the relativistic spin-orbit wave functions and compute observables such as the $\langle \mathbf{L}\cdot\mathbf{S} \rangle$ ground-state expectation value of the spin-orbit operator. The latter is in principle accessible from x-ray absorption and provides information on the role of t_{2g}–e_g couplings in the ground-state wave function and on the strength of non-cubic fields that lift the degeneracy of the t_{2g} levels. As concerns to the magnetic structure, we find, in honeycomb lattice structures, A_2IrO_3, the magnetic interactions strongly deviate from the proposed Kitaev-Heisenberg model, due to low-symmetry crystal fields.

O 41.10 Wed 13:00 H36

Bulk electronic structure of the diluted magnetic semiconductor GaMnAs through hard x-ray angle resolved photoemission — •Jan Minar[1], Igor diMarco[2], J. Braun[1], H. Ebert[1], A.X. Gray[3], and Ch. Fadley[3] — [1]University of Munich, Munich, Germany — [2]University of Upsalla, Upsalla, Sweden — [3]UC Davis, Davis, USA

A detailed understanding of the origin of the magnetism in diluted magnetic semiconductors is crucial to their development for applications. Using hard X-ray angle-resolved photoemission [1] at 3.2 keV, we investigate the bulk electronic structure of the prototypical diluted magnetic semiconductor GaMnAs, and the undoped reference system GaAs [2]. The fully self-consistent combination of LSDA and dynamical mean field theory (DMFT) [3,4] and its combination with the one-step model of photoemission has been used to explain the experimental findings. Distinct differences are found between angle-resolved, as well as angle-integrated, valence spectra of GaMnAs and GaAs, in good agreement with theory. In addition to the standard LSDA based calculations the LSDA+DMFT approach shows an important effect of electronic correlations on the states close to the Fermi level. The combination of LSDA+DMFT and corresponding the Monte-Carlo simulations indicates an origin of ferromagnetism in GaMnAs and provides us a rather unifying picture of this controversial material.

[1]A. Gray et al., J. Minar et al., Nat. mat. 10, 759 (2011) [2] A.

Gray, J. Minar et al., Nat. mat. 11, 957 (2012) [3] J. Minar, J. Phys.: Cond. Mat. (Topical Review) 23, 253201 (2011)

O 41.11 Wed 13:15 H36

Magnetic state of pyrochlore $Cd_2Os_2O_7$ emerging from strong competition of ligand distortions and longer-range crystal anisotropy — •Nikolay Bogdanov[1], Remi Maurice[2], Ioannis Rousochatzakis[1], Jeroen van den Brink[1], and Liviu Hozoi[1] — [1]IFW Dresden, Germany — [2]Groningen University, The Netherlands

We investigate the correlated *d*-level electronic structure of $Cd_2Os_2O_7$, a spin $S=3/2$ pyrochlore, by fully *ab initio* quantum-chemical many-body calculations on finite embedded clusters. The wave-function quantum-chemical methods provide a promising alternative to density-functional-based approaches to the electronic structure of solids. We describe the local Os d^3 multiplet structure, the precise mechanism of second-order spin-orbit coupling and zero-field splitting (ZFS), and determine the parameters of the effective spin Hamiltonian, i.e., the single-ion anisotropy, nearest-neighbor Heisenberg exchange as well as the Dzyaloshinskii-Moriya interactions.

The results indicate that local ligand distortions and the anisotropic Cd-ion coordination strongly compete, rendering the magnetic interactions and ordering crucially depend on these geometrical features. Without trigonal distortions a large easy-plane magnetic anisotropy develops. Their presence, however, reverses the sign of the ZFS and causes a large easy-axis anisotropy ($D \simeq -6.8$ meV), which in conjunction with the antiferromagnetic exchange interaction ($J \simeq 6.4$ meV) stabilizes an all-in/all-out magnetic order. The competition uncovered here is a generic feature of 227 pyrochlore magnets and opens new perspectives on the basic magnetism in these materials.

O 42: Organic/bio Molecules on Metal Surfaces IV

Time: Wednesday 10:30–13:15 Location: H38

O 42.1 Wed 10:30 H38

Modification of Cu(111) with buckybowls — •Quirin S. Stöckl[1], Tobias Bauert[1], Davide Bandera[2], Manfred Parschau[1], Jay S. Siegel[2], and Karl-Heinz Ernst[1,2] — [1]Empa, Nanoscale Material Science, Dübendorf, Switzerland — [2]Organisch-chemisches Institut, Universität Zürich, Switzerland

Interesting candidates for surface modifications for organic photovoltaics or controlled carbon nanotube growth are buckybowls, geodesic polyarenes and quasi-fragments of C_{60}. Corannulene (COR, $C_{20}H_{10}$) is the simplest curved fragment with a central pentagonal ring, surrounded by five aromatic C6 rings. Fivefold symmetry is incompatible with the translational order in all 17 plane groups, and this system is therefore of fundamental interest for 2D self-assembly. We have studied therefore the self-assembly of the star-like pentaphenyl-corannulene (Ph_5Cor) with STM. The packing motifs basically consist of anti-parallel rows with interdigitated substituents. Results will be compared to structures found for other penta-substituted COR derivatives and for monoindeno-corannulene.

O 42.2 Wed 10:45 H38

C_{58} on Au(111): an STM-based study — Noelia Bajales[1], Stefan Schmaus[1], Toshio Miyamachi[1], Wulf Wulfhekel[1], Jan Wilhelm[2], Melanie Stendel[2], Michael Walz[2], Alexej Bagrets[2], Ferdinand Evers[2], Seyithan Ulas[3], •Bastian Kern[1,3], Artur Böttcher[3], and Manfred M. Kappes[3] — [1]Institute of Physics, Karlsruhe Institute of Technology (KIT), Wolfgang-Gaede-Str. 1, D-76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [3]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

Non-IPR C_{58} cages were adsorbed at room temperature onto Au(111) by low-energy cluster beam deposition (E_{kin} 6 eV [1]). The surface topography and electronic properties of the system were investigated with a 4K-STM. The topographic images reveal that in the early adsorption stage (i.e. at low coverages), the cages are pinned by step edges and dislocation point defects and act as nucleation centers for growth of 2D islands. The isolated monomers exhibit no internal structure due to covalent bonding to the Au(111) surface. The short oligomers reflect a spontaneous surface-mediated polymerization of the cages. Dimers and trimers exhibit unique topographic features which reveal the covalent nature of the intercage bonds. The surface-independent outermost C_{58} layers appear to be wide band semiconductors (HOMO-LUMO gap 1.2 eV). Experimental results are compared with detailed DFT calculations.

O 42.3 Wed 11:00 H38

The molecular structure of a nine amino acid peptide at metal surfaces in vacuum — •Gordon Rinke[1], Stephan Rauschenbach[1], Rico Gutzler[1], Alyazan Albargash[1], Ludger Hanau[2], and Klaus Kern[1,3] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]Max-Planck Institute for Intelligent Systems, Stuttgart, Germany — [3]Institut de Physique de la Matiere Condensee, EPF Lausanne, Switzerland

Self-assembly of small molecules at surfaces in ultrahigh vacuum (UHV) is typically described as the interplay of intermolecular and molecule-surface interactions. Significant conformational changes or intramolecular interactions are rarely considered in this picture of self-assembly because these are relevant only for large molecules, which cannot be brought to surfaces in UHV by conventional deposition methods. The combination of electrospray ion beam deposition and scanning tunneling microscopy (STM) allowed us to study the molecular self-assembly of proteins and peptides in UHV.

In this study we address the self-assembly of Bradykinin (BK), a nine amino acid peptide with a mass of 1060u and large enough to interact with itself. Experimentally we find several conformations of BK in single molecule and dimer structures as well as in a superstructure of dimers. Conformations suggested by molecular dynamics simulations and calculated by density functional theory are compared to STM topographies and provide a tentative model of the adsorption.

Our study suggests that rationally synthesized peptides on surfaces can fold into structures with unique catalytic and chemical functions.

O 42.4 Wed 11:15 H38

Specific Material Binding by Peptide Motifs on the Oxidized Titanium and Silicon Surface — •Julian Schneider[1,2] and Lucio Colombi Ciacchi[1] — [1]Hybrid Materials Interfaces Group, Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Department Chemie, Technical University Munich, Germany

The specific recognition of materials surfaces by small peptide sequences has become a widely investigated, interdisciplinary research topic with fields of application ranging from bio-nanotechnology to medicine and pharmacology [1]. However, a rationalization of the binding driving forces in terms of a clear structure-function relationship is missing, as the atomistic details of material surfaces in a wet environment are hard to elucidate both experimentally and theoretically.

Using a combination of metadynamics, replica exchange and steered molecular dynamics simulations we unveil the origin of the selectivity of specific binding motifs for Ti over Si, obtaining adsorption free energies and adhesion forces in quantitative agreement with corresponding experiments. We present evidence that the observed material recognition by small peptides is governed by local solvent density variations at solid/liquid interfaces, sensed by the side-chain residues with atomic-scale precision [2].

[1] M. Sarikaya, C. Tamerler, A. K.-Y. Jen, K. Schulten, and F. Baneyx. *Nature Mater.*, **2**, 577 (2003).

[2] J. Schneider and L. Colombi Ciacchi. *J. Am. Chem. Soc.* **134**, 2407 (2012).

O 42.5 Wed 11:30 H38

Chemical Transformations of Bisphenol A on Cu(111) and Ag(111) — •Julian Lloyd, Sybille Fischer, Anthoula Papageorgiou, Matthias Marschall, Joachim Reichert, Katharina Diller, Florian Klappenberger, Francesco Allegretti, and Johannes V. Barth — Physik Department E20, TUM, Garching

Bisphenol A (BPA) is a common additive to everyday polymers and its suspected adverse health effects led to its EU ban from use in baby bottles in June 2011. Some of these effects are traced to DNA alterations [1]. The reactivity of BPA has not been reported in a systematic way and the key molecular events and interactions driving the self-assembly of non-coplanar phenols have hitherto not been addressed unambiguously by a combinatorial approach of microscopy and spectroscopy. In this study we address the chemical transformations of BPA on transition and noble metal surfaces, copper and silver. These transformations are expected to induce changes in the surface self-assembly. Performing a scanning tunneling microscopy study of BPA on a Cu(111) and a more inert Ag(111) surface we observed multiple extended two dimensional networks dependent on temperature and substrate metal. To further elucidate the chemical state and the orientation of the molecule in the aforementioned phases, we performed synchrotron X-ray photoelectron spectroscopy and near-edge X-ray absorption fine structure studies. We find a complex, stepwise deprotonation scheme mediating the structural transformations. Based on the data sets we present a simple comprehensive model of the observed phases.

[1] D.C. Dolinoy, et. al. PNAS 104, 13061 (2007).

O 42.6 Wed 11:45 H38

Diethylstilbestrol on Ag(111) and Cu(111): an STM study — •Seung Cheol Oh, Julian A. Lloyd, Sybille Fischer, Özge Altuntasoglu Saglam, Anthoula C. Papageorgiou, Joachim Reichert, and Johannes V. Barth — Physik Department E20, Technische Universität München, 85748 Garching, Germany

Diethylstilbestrol (DES) is a synthetic estrogen, which has been banned after its association with adverse health effects. It contains two phenol groups, which can be coplanar, thus allowing the molecule to act as ditopic surface molecular linker. Our study was motivated by the fact that phenol groups can be used to control of molecular self-assembly [1]. Here we focus on investigating the self-assembly of DES on two single crystal metal surfaces by means of variable-temperature scanning tunneling microscopy (STM). We find a variety of different two-dimensional molecular networks depending on the supporting metal (silver and copper) and on the annealing temperature. Based on the known interactions of phenols on surfaces as well as a carefull analysis of STM topographic images we present tentative strucural models for the observed self-assembled nanosctructures.

[1] Pawlak, R. et al. *ChemPhysChem* **2009**, *10*, 1032–1035.

O 42.7 Wed 12:00 H38

Initial growth of quinacridone on Ag(111) — •Thorsten Wagner, Michael Györök, Daniel Huber, and Peter Zeppenfeld — Johannes Kepler University, Institute of Experimental Physics, Linz, Austria

The organic dye pigment quinacridone (QAC) may play a role as an outsider in view of record breaking organic semiconductors like rubrene, but its dominant H-bonds might be a key to innovative device structures. Therefore, this work focusses on the initial growth of quinacridone on Ag(111) surfaces at room temperature. During deposition, the local electron yield was monitored in a photoelectron emission microscope (PEEM) showing no spatial inhomogeneities on a scale between 100 nm and 100 μm for up to 5 monolayers. This could be either due to a smooth layer-by-layer growth or the formation of extraordinary small 3D crystallites. The initial increase of the yield can be attributed to a lowering of the work function upon formation of the first monolayer. As the ionization potential of QAC (5.4 eV [1]) is actually higher than the photon energy (4.9 eV), a continuous decrease even below the emission of the bare Ag(111) substrate was observed afterwards. Scanning tunneling microcopy images of the initial layer exhibit a simple, raw-like stacking of parallel molecules which can be explained by hydrogen bonding between adjacent, flat-lying molecules. After annealing to a temperature of T=550-570 K, which is close to the desorption temperature of the multilayer, the structure changes to a stacking of dimers. Additional LEED data support the STM findings.

[1] Glowacki et al. in Applied Physics Letters 101, 023305 (2012)

O 42.8 Wed 12:15 H38

Different behaviour of Hydrogenated vs. Fluorinated Tribromobenzene on Ag(111) and Cu(111): the influence of pendant groups — •Stefan Schlögl[1,2], Wolfgang M. Heckl[1,2], and Markus Lackinger[1,2] — [1]Department of Physics & TUM School of Education, Tech. Univ. Munich, Schellingstrasse 33, 80333 Munich, Germany — [2]Deutsches Museum, Museumsinsel 1, 80538 Munich, Germany

A lot of effort has been put into the realization of the dream of two-dimensional polymers. Bottom-up fabrication of 2D polymers facilitates tailoring of desired electrical, thermal and mechanical properties for new classes of materials and semiconductors.[1] To gain further knowledge about on-surface reactions of 2D polymers, a systematic study of the influence of pendant groups an the self-assembly and polymerization process has been performed. Pendant groups are known to alter physical and electrochemical properties of synthesized polymers.[2] Here we compare the polymerization of s-tribromobenzene derivatives either hydrogenated or perfluorinated on two surfaces. Therefore, 1,3,5-Tribromo-2,4,6-Trifluoro-benzene and 1,3,5-Tribromobenzene were deposited onto Ag(111) and Cu(111) and characterized by means of scanning tunneling microscopy under ultra-high vacuum conditions. Reaction mechanisms to describe the different behavior of the two monomers are proposed.

[1] Sakamoto, J. et al., Angew. Chem., Int. Ed., 48 (2009), Nr. 6, 1030-1069. [2] Wang, Z. et al., J. Membrane Sci., 285 (2006), Nr. 1-2, 239-248.

O 42.9 Wed 12:30 H38

Synthesis of 2D covalent networks through Ullmann coupling of a threefold symmetric hexabrominated molecule — •Atena Rastgoo Lahrood[1,2], Thomas Sirtl[1,2], Wolfgang Heckl[1,2], and Markus Lackinger[1,2] — [1]Department of Physics & TUM School of Education, Tech. Univ. Munich, Schellingstrasse 33, 80333 Munich, Germany — [2]Deutsches Museum, Museumsinsel 1, 80538 Munich, Germany

Over the last few years, 2D covalent materials have gained a lot of interest in different fields of studies because of their extraordinary properties. One of the common bottom-up synthesis methods for 2D covalent networks is surface mediated polymerization of halogenated organic monomers. Thereby, surface stabilized radicals are generated through the homolysis of carbon-halogen bonds. Subsequent diffusion and radical recombination reactions yield covalently cross-linked networks. In this contribution we will discuss the role of the monomer halogen substitution pattern for the topology and defect density in covalent networks. Moreover, comparative studies on densely packed coinage metal surfaces (Cu(111), Ag(111), Au(111)) and additional thermal treatment reveal the influence of further important parameters. The structures are prepared in ultra-high vacuum and analyzed by STM and LEED. Molecules were also deposited onto Ag(111) and Cu(111) at low temperature and structural changes that hint toward the onset of polymerization were studied as a function of temperature.

O 42.10 Wed 12:45 H38

Unconventional self-assembled monolayers with unusual properties — David A. Egger[1], Ferdinand Rissner[1], Oliver T. Hofmann[1], Amir Natan[2,3], Leeor Kronik[2], Georg Heimel[4], and •Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, 8010 Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, 76100 Rehovoth, Israel — [3]Department of Physical Electronics, 69978 Tel-Aviv University, Tel-Aviv, Israel — [4]Institut für Physik, Humboldt-Universität zu Berlin, Brook-Taylor-Straße 6, 12489 Berlin, Germany

We use density-functional theory calculations to show that self-assembled monolayers (SAMs) made from molecules consisting of conjugated distributed dipolar units have unusual properties: * Work-function modifications tuned linearly with the number of repeat units are limited by Fermi-level pinning,[1] where the limitations can be overcome using advanced design strategies.[2] * Collectively induced internal electric fields change the nature of the electronic states within such SAMs in a way strongly reminiscent of the quantum-confined Stark-effect [3] with a closure of the global band-gap beyond a certain number of repeat units. [4] * Moreover, SAMs can be realized that display different polarity of charge transport, in spite of consisting of molecules with virtually identical electronic properties.[5] All these observations can be traced back to collective effects prevalent in such SAMs. [1] Phys.Chem.Chem.Phys., 2010, 12, 4291; [2] Nano Lett. 10, 4369 (2010); [3] J. Am. Chem. Soc. 133, 18634 (2011); [4] Org. El. 13, 3165 (2012); [5] Adv. Mater. 24, 4403 (2012).

O 42.11 Wed 13:00 H38

Control of Intermolecular Bonds by Deposition Rates: Hydrogen Bonds vs. Metal-Coordination in Trinitrile Monolayers — •Thomas Sirtl[1,2], Stefan Schlögl[1,2], Atena Rastgoo-Lahrood[1,2], Jelena Jelic[3], Subhadip Neogi[4], Michael Schmittel[4], Wolfgang M. Heckl[1,2,5], Karsten Reuter[3], and Markus Lackinger[2,5] — [1]Department of Physics, Tech. Univ. Munich, James-Franck-Str. 1, 85748 Garching — [2]Center for NanoScience

(CeNS), Schellingstr. 4, 80799 Munich — [3]Department of Chemistry, Tech. Univ. Munich, Lichtenbergstr. 4, 85747 Garching — [4]Center of Micro- and Nanochemistry and Engineering, Organische Chemie I, Universität Siegen, Adolf-Reichwein-Str. 2, 57068 Siegen — [5]Deutsches Museum, Museumsinsel 1, 80538 Munich (all Germany)

Self-assembled monolayers of a large functional trinitrile molecule are studied on the (111) surfaces of copper and silver by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). A densely packed hydrogen bonded polymorph was equally observed on both surfaces. Additionally, deposition onto Cu(111) yielded a well-ordered metal-coordinated porous polymorph that coexisted with the hydrogen bonded structure. The coordination centers are supplied by the adatom gas of Cu(111). On Ag(111) the metal-coordinated network was never observed. Differences in the adatom reactivity and the resulting bond strength are held responsible for this substrate dependence. By utilizing ultra-low deposition rates, we demonstrate that on Cu(111) adatom kinetics plays a decisive role in the expression of intermolecular bonds - and hence for structure selection.

O 43: Plasmonics and Nanooptics IV

Time: Wednesday 10:30–13:15 Location: H31

O 43.1 Wed 10:30 H31

Repetitive hole-mask colloidal lithography for large-area multi-shape plasmonic nanostructures — •Jun Zhao[1], Sarah Jaber[2], Paul Mulvaney[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]School of Chemistry and Bio21 Institute, University of Melbourne, Australia

We fabricate large-area (cm2 size) plasmonic nanostructures of multiple shapes, orientations, and sizes. We utilize repetitive hole-mask colloidal lithography with sparsely distributed polystyrene beads. Multiple lithography leads to neat structures with high area coverage and very little nanostructure touching or overlap. The optical spectra of our sample show well modulated resonances, which confirm the high quality of our fabrication method. Our method is useful to create polarization-independent split-ring arrays, broadband multi-peak infrared antennas for SEIRA enhancement[1], nanostructures with simultaneous SERS and SEIRA enhancement in the visible and IR, as well as chiral 3D plasmonic structures with C3 or C4 symmetry.

[1] S. Cataldo, J. Zhao, F. Neubrech, B. Frank, C. Zhang, P. V. Braun, H. Giessen, ACS Nano 2012, 6, 979.

O 43.2 Wed 10:45 H31

Plasmonic Sensing using Hydrogen induced Phase Transitions in Yttrium Nanoparticles — •Nikolai Strohfeldt[1], Andreas Tittl[1], Frank Neubrech[1], Uwe Kreibig[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center Scope, University of Stuttgart, D-70550 Stuttgart, Germany — [2]I. Physikalisches Institut 1A der RWTH Aachen, D-52056 Aachen, Germany

We utilize the subsequent hydration of Yttrium nanoparticles [1] to construct an extremely sensitive optical hydrogen detector. Upon the reaction pathway $Y \rightarrow YH_2 \rightarrow YH_3$ the material undergoes two phase transitions. The second transition from the metallic YH_2 to the dielectric YH_3 is reversible at room temperature and therefore highly interesting for hydrogen sensing applications. Our lithographically defined 50 nm thick and 200 nm diameter nanoparticles exhibit a strong and sharp particle plasmon resonance in the metallic YH_2 state. Upon exposure with 4% H_2 in N_2, within seconds the particle plasmon absorption vanishes completely as the particles undergoes a reversible metal-to-insulator phase transition to YH_3. This large relative change will enable the construction of novel, ultra-sensitive, optical, single-nanoparticle hydrogen sensors in the future.

[1] G. Bour, A. Reinholdt, A. Stepanov, C. Keutgen, and U. Kreibig, "Optical and electrical properties of hydrogenated yttrium nanoparticles," The European Physical Journal D **16**, 219-223 (2001).

O 43.3 Wed 11:00 H31

Detecting low concentrations of pollutant chemicals in water by SERS:Combining optimised nanoparticle ensembles and SERDS — •Robert Ossig[1], Yong-Hyok Kwon[2], Heinz-Detlef Kronfeldt[2], and Frank Hubenthal[1] — [1]Institut für Physik and CINSaT, Universität Kassel, Germany — [2]Technische Universität Berlin, Institut für Optik und Atomare Physik, Germany

We present a sensor that is suitable to detect very low concentrations of pollutant chemicals, e.g. polycyclic aromatic hydrocarbons (PAHs). To meet the European Quality Standard (EQS) criteria for PAHs, which require limits of detection (LOD) in the sub nMol/l regime, we combined surface enhanced Raman spectroscopy (SERS) with shifted excitation Raman difference spectroscopy (SERDS) and used supported noble metal nanoparticles (NPs) as SERS substrates. The NPs were prepared by Volmer-Weber growth under ultra high vacuum conditions. To gain optimal SERS enhancement the NPs plasmon resonance positions were tuned to coincide with the excitation wavelengths for SERDS. We demonstrate that our sensor using bare NPs yield LODs between 2 and 4 nMol/l, sufficient to detect the maximum allowable concentration of PAHs in water, as determined by the EQS. Furthermore we can reliably detect these concentrations in about 10 minutes. However, the annual average concentration requires LODs below the nMol/l regime. To reliably detect such low concentrations the functionalization of the NPs is currently under investigation. The functionalization enhances the adsorption of probe molecules to the NPs, which leads to a further improvement of the LOD.

O 43.4 Wed 11:15 H31

Strong SERS Enhancement Based on Large Area Controllable Gold Nanoparticle Arrays with High Uniformity and Reproducibility — •Yan Zheng, Chengliang Wang, Wenxin Wang, Felix Stosberg, and Yong Lei — Fachgebiet 3D-Nanostrukturierung, Institut fuer Physik & IMN MacroNano, Technische Universitaet Ilmenau, Germany

Significant SERS (surface enhanced Raman Scattering) enhancement with uniformity and reproducibility are achieved based on controllable highly ordered gold nanoparticle arrays, which can be obtained in large area by using ultra-thin alumina membranes (UTAMs) as shadow masks[1-2]. By controlling the anodization process, the pore-widening period of UTAM masks and the thermal deposition of nanoparticles, ordered Au nanoparticle arrays with different diameter and different surface morphology were obtained[3]. The Raman spectra of the Au nanoparticle arrays suggest that rough surface morphology can facilitate the SERS effect and the optimum diameter of nanoparticles is about 55 nm. All the results indicate that the template-prepared highly ordered Au nanoparticles on Si wafers with reproducible homogeneous SERS signals are high performance SERS substrates, which shall have important applications for SERS-related devices.

[1] Lei Y., Yang S.H., Wu M.H., Wilde G., Chemical Society Reviews, 40(3), 1247-1258, 2011. [2] Yang S.K., Cai W.P., Kong L.C., Lei Y., Advanced Functional Materials. 20(15), 2527-2533, 2010. [3] Wen L.Y., Wu M.H., Ostendorp S., Chen K., Wilde G., Lei Y., Small, 6(5), 695-699, 2010.

O 43.5 Wed 11:30 H31

Fabrication of plasmonic Ag/Au arrays used as sensitive platform for glucose assay — •Wenxin Wang, Yan Zheng, Ahmed Shukur Hameed Al-Haddad, Yan Mi, Huaping Zhao, and Yong Lei — Fachgebiet 3D-Nanostrukturierung, Institut fuer Physik & IMN MacroNano (ZIK), Institute for Physics and IMN MacroNano (ZIK), Technische Universitaet Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany.

A noble Ag/Au plasmonic array used for glucose detection based on enzyme-responsive was first obtained. Such kind of Ag arrays stands on the Au covered substrate which connected with glucose oxide (GOx) was prepared via mutli-steps physical vapor deposition combined with ultra-thin anodic alumina membranes. When the GOx from the substrate meeting with glucose, the produced H2O2 will etching origin Ag array into porous that will induce the variation of its optical property. Because plasmon resonance is sensitive to the structure, therefore with this new platform, even a little glucose can quickly detected from the shifting of extinction spectrum. We believe this king of glucose sensing platform has bright future in commercial application.

O 43.6 Wed 11:45 H31

Plasmonic Smart Dust for Probing Local Chemical Reactions

— •Andreas Tittl^1, Xinghui Yin^1, Harald Giessen^1, Xiang-Dong Tian^2, Christian Kremers^3, Dmitry N. Chigrin^3, Zhong-Qun Tian^2, and Na Liu^4 — ^{1}4th Physics Institute and Research Center Scope, University of Stuttgart — ^{2}State Key Laboratory for Physical Chemistry of Solid Surfaces and Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University — ^{3}Institute of High-Frequency and Communication Technology, Faculty of Electrical, Information and Media Engineering, University of Wuppertal — ^{4}Max Planck Institute for Intelligent Systems, Stuttgart

We demonstrate an all-optical probing technique based on plasmonic smart dust for monitoring local chemical reactions in real time. Our smart dust consists of silica shell-isolated gold nanoparticles which can work as strong light concentrators and optically report subtle changes at their pinning sites on the probed surface during reaction processes. In particular, we investigate the hydrogen dissociation and subsequent absorption in neighboring palladium films with both „dust-on-film“ and „film-on-dust“ platforms. Our single particle scattering measurements illustrate the ability of this technique to optically resolve chemical reactions while they occur on various surface morphologies. The presented technique offers a unique scheme for real-time, label-free, and high-resolution probing of local reaction kinetics in a plethora of chemical reactions on surfaces.

O 43.7 Wed 12:00 H31

Label-free single-protein optical sensing and imaging — •Marek Piliarik and Vahid Sandoghdar — Max Planck Institute for the Science of Light Günther-Scharowsky-Str. 1, Building 24 91058 Erlangen, Germany

To date, the sensitivity of optical detection and imaging of individual molecules is strictly limited to species with strong fluorescence or absorption properties. We report on a new approach based on the direct detection of the light scattered by biomolecular species such as proteins without the need for any labels. The underlying mechanism of our detection method is the interference between the light coherently scattered by the analyte (e.g. a protein molecule adsorbed on the substrate) and the laser beam partially reflected at the substrate-water interface. By combining this method with microfluidics and surface functionalization of the substrate, we show that it is possible to detect and image a single protein in real time and distinguish it from a large background of other scatterers. We discuss the application of our approach for ultrasensitive label-free biosensing.

O 43.8 Wed 12:15 H31

Voltage clamped single gold nanoparticles as nanoscale pH-sensors — •Cynthia Vidal^1, Martin Djiango^1, Calin Hrelescu^1, Thomas A. Klar^1, Andrei I. Mardare^2, and Achim Walter Hassel^2 — ^{1}Institute of Applied Physics, — ^{2}Institute for Chemical Technology of Inorganic Materials, Johannes Kepler University, 4040 Linz, Austria

The surface chemistry of gold nanoparticles plays a crucial role when used in biodiagnostics, in surface enhanced Raman scattering and catalysis. The processes of double layer charging, increased damping of the plasmons due to adsorbates, and oxidation of single gold nanorods were recently investigated by optical dark field spectroscopy of voltage-clamped single gold nanoparticles [1,2]. In this work, the pH-dependence of the reversible formation/reduction of hydrous gold oxide layers on a single nanoparticle was investigated by combining electrochemistry with monitoring the plasmon resonance of single gold nanorods in a dark field microscope. Changing from an acidic environment to a more basic one, a shift of the hydrous oxide reduction point to lower potentials is observed. In combination with cyclic voltammetry results, the spectral shifts of the nanoparticle plasmon resonance can be correlated with these phenomena. The presented combination of electrochemistry and optical spectroscopy at a single nanoparticle level allows for the use of single gold nanoparticles as nanoelectrodes, providing a novel tool for electrochemistry and electro catalysis on the nanoscale. [1] Nano Lett. 12, 1247 (2012) [2] Nanoscale 4, 2339 (2012)

O 43.9 Wed 12:30 H31

Broadband subwavelength imaging using a tunable graphene-lens — •Peining Li and Thomas Taubner — RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany

Graphene as a one-atom-thick planar sheet can support surface plasmons at infrared (IR) and terahertz (THz) frequencies, opening up exciting possibilities for the emerging research field of graphene plasmonics. Here, we theoretically report that a layered graphene-lens (GL) enables the enhancement of evanescent waves for near-field subdiffractive imaging [1]. Compared to other resonant imaging devices like superlenses [2,3], the nonresonant operation of the GL provides the advantages of a broad intrinsic bandwidth and a low sensitivity to losses, while still maintaining a good subwavelength resolution of better than $\lambda/10$. Most importantly, thanks to the large tunability of the graphene, we show that our GL is a continuously frequency-tunable subwavelength-imaging device in the IR and THz regions, thus allowing for ultrabroadband spectral applications.

[1] P. Li, T. Taubner, ACS Nano, In press.

[2] J. B. Pendry, Phys. Rev. Lett., 85, 3966-3969, (2000).

[3] T. Taubner et. al., Science, 313, 1595-1595, (2006).

O 43.10 Wed 12:45 H31

Antenna-enhanced infrared near-field nanospectroscopy of a polymer — •Jón Mattis Hoffmann, Benedikt Hauer, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany

Infrared spectroscopy is a powerfull characterization tool which allows for the investigation of chemical properties of a sample by directly probing molecular vibrations. On nanometer scale this is enabled by scattering-type scanning near-field optical microscopy (s-SNOM). This technique provides information about topographical and chemical material properties with subwavelength resolution.[1]

In this work, we demonstrate that the sensitivity of s-SNOM can be improved by means of infrared resonant antennas. This is comparable to the application of resonant nanostructures in far-field surface-enhanced infrared spectroscopy (SEIRS).[2] Here, antennas prepared with colloidal lithography are used to enhance the spectra of a polymer coverlayer. We find that the near-field amplitude spectra of the polymer obtained on resonant structures are increased in absolute value as well as in contrast over those obtained on non-resonant, highly reflective materials such as gold.[3]

[1] F. Keilmann et al. in Nano-Optics and Near-Field Optical Microscopy ed. by A. Zayats and D. Richards, 235 (ArtechHouse, 2009).

[2] F. Neubrech et. al., Physical Review Letters 105, 157403 (2008).

[3] J. M. Hoffmann et. al., Applied Physics Letters 101, 193105 (2012).

O 43.11 Wed 13:00 H31

Raman spectra of individual carbon nanotubes manipulated by surface plasmons — •Nicola Paradiso, Fatemeh Yaghobian, Tobias Korn, Christian Schüller, and Christoph Strunk — Institut für Experimentelle und Angewandte Physik, Universität Regensburg.

The Raman spectrum of individual carbon nanotubes (CNTs) can be enhanced by noble metal nanoparticles, due to surface-enhanced Raman scattering (SERS). In this work we exploit lithographically patterned nanoparticles to locally obtain SERS from the desired position along a CNT. Such structures consist of arrays of sharp triangular metal pads separated by a 20 nm-wide gap, which are fabricated via electron beam lithography. AFM scans allow us to align the lithography so that the CNT is lying within the gap between two nanostructures. When illuminated with the Raman source, surface-plasmons are generated at the surface of these gap sized engineered structures. This method allows us to separately characterize electromagnetic and the chemical contributions in SERS. In particular, we have analyzed how the presence of noble metal structures manipulates the radial breath mode in the spectrum, and how the G+/G- amplitude ratio is locally modified. Such an “on-chip” optical interface will make it possible to manipulate the optical features of the CNTs and allow to directly assigning the chirality of given individual CNTs.

O 44: Scanning Probe Methods I

Time: Wednesday 10:30–13:15 Location: H33

O 44.1 Wed 10:30 H33

Tuning Fork Sensor Spring Constants and Q-Factors in Experiment and Simulation — •Marvin Stiefermann[1], Jens Falter[2], Harald Fuchs[2], and André Schirmeisen[1] — [1]Universität Gießen — [2]Universität Münster

The increasing application of Tuning Fork (TF) based sensors in noncontact Atomic Force Microscopy (nc-AFM) raised the need for a comprehensive investigation of the two most relevant sensor parameters, the spring constant and Q-factor. Those sensors were primarily designed for the application in watches, and the change of these parameters when mounted in the AFM setups is not well understood. In this work we performed detailed measurements and finite element simulations to understand and determine the TF spring constants as well as Q-factors for different mounting geometries. With a specially developed setup, consisting mainly out of a micrometer caliper and a high sensibility scale, it was possible to apply different forces along arbitrary positions of the prong of the TF, which was attached onto a Macor block holder. Reliable results were achieved only by applying compressive and tensile forces to the TF, allowing us to eliminate the contribution of the tungsten tip deformation to the spring constant. In a second step the complete experimental setup was rebuilt in a finite-element computer model, including the glue points, tip mass and position as well as the Macor holder geometry. This model is in quantitative agreement with the experimental results for the spring constant and allows us to identify the critical parameters to obtain a high Q- factor.

O 44.2 Wed 10:45 H33

Friction induced self-excited cantilever resonance oscillation — •Felix Mertens, Thomas Göddenhenrich, and André Schirmeisen — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392 Gießen

The modulation of a sample in the direction of the cantilever long axis leads to bending oscillations of the lever if the tip is in contact with the surface[1]. The lever response oscillation essentially depends on the modulation amplitude and the modulation frequency. Experimental and simulated data indicate that a modulation frequency well below the resonance frequency of the lever and a sufficient modulation amplitude for stick-slip motions of the tip causes a lever response oscillation containing the modulation frequency as well as the self-excited bending resonance frequency of the lever. [1]T. Göddenhenrich, S. Müller, and C.Heiden, Rev. Sci. Instrum. 65, 2870 (1994)

O 44.3 Wed 11:00 H33

Investigations on nanocantilever dynamics in intermittent-contact AFM — •Moid Bhatti, Ivo Knittel, Uwe Schmitt, Andreas Englisch, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, 66041 Saarbruecken, Germany

High speed (video rate and beyond) atomic force microscopy (AFM) requires not only fast feedback with a bandwidth exceeding 100 kHz - for which solutions are emerging - but also cantilever resonant frequencies in the MHz range. Nanocantilevers (NC) can fulfill this requirement motivating an understanding of the NC-sample interaction.

We are studying contact mechanics of the cantilever-sample system in the dynamic mode AFM using NC of various types: (1) nanowires (NW) grown on a substrate (the dynamic behavior of which is equivalent to a cantilever with a NW attached to it), (2) carbon nanotubes attached to an AFM cantilever, (3) focused-ion-beam-(FIB)-structured NC, (4) a FIB-structured NC at the tip of an optical fiber, whereby the light transmission capability of the fiber can be utilized for the integrated detection of the NC oscillation.

We will present different NC, FEM simulations of NC resonances, a detection mechanism and AFM imaging with NC. The contact stiffness with NC can be very low resulting in a characteristic tip-sample force-distance relation. Distance-dependent resonance curves of an AFM cantilever interacting with a static NW and of a NC tapping on a sample showing the existence of a third state of cantilever dynamics besides the well-known "low- and high-amplitude" states will be presented including the effect of adhesion and dissipation.

O 44.4 Wed 11:15 H33

Development of a Quattro-Cantilever Microscope for topological and electrical measurements — Robert Benzig[1], Marcus Kästner[1], Tzvetan Ivanov[1], Manuel Hofer[1], •Anne-D. Müller[2], Falk Müller[2], and Ivo W. Rangelow[1] — [1]TU Ilmenau, Fakultät für Elektrotechnik und Informationstechnik, Institut für Mikro- und Nano-Elektronik, 98693 Ilmenau, Germany — [2]Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz/V., Germany

In the past 15 years, extended developments of AFMs continually have involved multiple cantilever designs that allow the simultaneous operation of more than one AFM tip with the aim to speed up the image acquisition or to use different tips for different purposes [1]. This contribution introduces a thermally driven self-sensing four cantilever array and its application based on an extendable experimental set-up. Each cantilever is operated with an independent dynamic mode feedback while the vertical movement range is about 1.2 μm and connected to dedicated feedback loops. In addition, a master feedback loop operates a standard AFM scanner with 5 μm vertical range. The contribution explains the technical details of the cantilever array, fabrication technology and the experimental set-up. We will demonstrate the simultaneous operation of all four cantilevers (so-called Quattro-Cantilever-Chip).

O 44.5 Wed 11:30 H33

Technical limitations in dynamic mode high-speed AFM imaging — •Anne-D. Müller and Falk Müller — Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz, Germany

As the availability of AFM probes and digital control technology have improved substantially within the past decade, high-speed imaging in contact and dynamic mode AFM became an achievable goal for current instrumentation development. In order to reasonably track the topology of the surface, the most important target of current investigations is the response time of the digital feedback loop. This contribution presents a technical solution for the direct determination of the frequency dependent disturbance rejection of digital feedback loops considering the whole system including the cantilever, the lockin amplification and all required A/D and D/A converters. It will be shown that the cantilever itself remains as bottleneck for the further increase of the imaging speed in dynamic mode. Results acquired with different commercially available high-speed cantilevers will be compared.

O 44.6 Wed 11:45 H33

Conductive AFM for characterization of MW-CNT-based via interconnect systems — •Marius Toader[1], Holger Fiedler[2], Sascha Hermann[2], Stefan E. Schulz[2,3], Thomas Gessner[2,3], and Michael Hietschold[1] — [1]Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — [2]Chemnitz University of Technology, Center for Microtechnologies, D-09126 Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems (ENAS), D-09126 Chemnitz, Germany

Advanced hybrid interconnects where copper will be replaced using carbon nanotubes (CNTs) will represent the breakthrough in overcoming the actual limitations of interconnect industry strongly constrained by the shrinking issues. To successfully proceed with the development and improvement of such systems, a comprehensive understanding is required and therefore a detailed characterization should be addressed. We report on and emphasize the versatility of conductive AFM (c-AFM) in characterizing vertically aligned CNTs aimed to be used in via interconnect technology. The study is conducted on multi-walled CNT (MW-CNT) arrays vertically grown on a copper-based metal line [1]. The advantages of the c-AFM with respect to the classical electrical measurements are discussed. A detailed insight into the internal performance is achieved via current-voltage spectroscopy. [1] Fiedler H, Toader M, Hermann S, Rodriguez R, Sheremet E, Rennau M, Schulze S, Waechtler T, Hietschold M, Zahn D, Schulz S, Gessner T: ECS Journal of Solid State Science and Technology 2012, 1(6) M47-M51.

O 44.7 Wed 12:00 H33

Passing current through molecular wires of different length — •Norman Fournier[1,2], Christian Wagner[1,2], Ruslan Temirov[1,2], and Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]JARA-Fundamentals of Future Information Technology

Recently we developed a method to contact a single molecule on a metal substrate and lift it up with the tip of a combined AFM/STM based on the qPlus sensor [1]. While lifting, we pass the current through the molecule and measure the conductance. The geometry of the junction is controlled by measuring the frequency shift of the qPlus sensor [2].

We applied this method to a set of π-conjugated molecules of different length which all have the same anchoring group. By doing this systematically we probed the transport properties of the wire depending on its length. We also investigated how the transport through the molecule depends on its contacts by using two differnet types of electrodes (Ag and Au).

References

[1] N. Fournier et al. Physical Review B 84, 035435 (2011)

[2] C. Wagner et al. Physical Review Letters 109, 076102 (2012)

O 44.8 Wed 12:15 H33

Calibrating atomic-scale force sensors installed at the scanning tunneling microscope tip apex — Georgy Kichin[1,2], Christian Wagner[1,2], Stefan Tautz[1,2], and •Ruslan Temirov[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]JARA-Fundamentals of Future Information Technology

Using the combined low-temperature atomic force and scanning tunneling microscope (LT AFM/STM) we perform simultaneous force and conductance measurements on STM tips decorated with either a single carbonmonoxide molecule or an individual xenon atom. Our results show that both tips act as force sensors coupling the tunneling conductance of the junction to the force acting on the tip. On the basis of the obtained data we attempt the quantitative calibration of the observed sensor function.

O 44.9 Wed 12:30 H33

Capillary forces between a rigid sphere and an elastic half -space: the role of Young's modulus and equilibrium vapor adsorption — Marjan Zakerin[1], •Michael Kappl[1], Ellen Backus[1], Hans-Jürgen Butt[1], and Friedhelm Schönfeld[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz — [2]Hochschule RheinMain, Faculty of Engineering, Am Brückweg 10, 65428 Rüsselsheim

Capillary adhesion of microparticles to a deformable substrate was analytically calculated, simulated by finite element simulations and measured with an atomic force microscope. The effects of elastic deformation and liquid adsorption were analyzed. Using an atomic force microscope, we measured the force between a silica bead of 2 μm radius and a silicon wafer (Young's modulus E = 170 GPa) and polydimethylsiloxane (PDMS, E = 1 MPa) in the presence of ethanol at different vapor pressures. Adhesion forces on soft surface were much stronger than on rigid samples. In order to fully explain the experimental results, the previous developed theory by Butt et al. (1) was extended to take into account vapor adsorption of ethanol. Calculations were compared to results of finite element (FEM) simulations taking the detailed deformation of the elastic support close the meniscus explicitly into account.

(1) H.-J. Butt, W. J. P. Barnes, A. del Campo, M. Kappl and F. Schönfeld, Soft Matter, 2010, 6, 5930

O 44.10 Wed 12:45 H33

Efficient orbital dependent STM simulation model — •Gabor Mandi, Laszlo Szunyogh, and Krisztian Palotas — Budapest University of Technology and Economics, Department of Theoretical Physics, Budapest, Hungary

The interplay of experiment and theory is essential for the correct interpretation of experimental scanning tunneling microscopy (STM) results. We propose an orbital dependent tunneling model and implement it within an atom superposition approach for simulating STM [1].

In order to demonstrate the applicability of this method we consider a W(110) surface, and analyze the orbital contributions to the tunneling current and the corrugation of constant current STM images. In accordance with a previous study [2] we find atomic contrast reversal depending on the bias voltage. We analyze this effect depending on the tip-sample distance using different tip models and find two qualitatively different behaviors. As an explanation we highlight the role of the real space shape of the orbitals involved in the tunneling. STM images calculated by our model agree well with Tersoff-Hamann and Bardeen results. The computational efficiency of our model is remarkable as the k-point samplings of the surface and tip Brillouin zones do not affect the computation time, in contrast to the Bardeen method.

This research was supported by the OTKA PD83353, K77771, TAMOP-4.2.2.B-10/1-2010-0009 projects, and a Bolyai Grant.

[1] Palotas et al., arXiv:1206.6628 (2012).

[2] Heinze et al., Phys. Rev. B 58, 16432 (1998).

O 44.11 Wed 13:00 H33

Fundamental relation between chemical force and tunneling current driven by quantum degeneracy — Yoshiaki Sugimoto[1], Martin Ondráček[3], Masayuki Abe[1], Seizo Morita[1], Pablo Pou[2], Rubén Pérez[2], Fernando Flores[2], and •Pavel Jelínek[3] — [1]Graduate School of Engineering, Osaka University 2-1, Yamada-Oka, Suita, Osaka 565-0871, Japan — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049, Spain — [3]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10/112, Prague, 162 00, Czech Republic

Both the tunneling current I and the short-range component of the force F, induced by the formation of the chemical bond, exhibit in atomic contacts an exponential decay with similar characteristic decay length. Consequently, the relation between F and I follows the relation F^n I, where n is an integer number. Over the last 10 years, several different factors n have been proposed by different groups based on both theoretical analysis and experimental measurements; still there is no consensus on the relation between F and I.

We explain origin of two characteristic scaling regimes, where the current is either proportional to the force I∼F or to the square of the chemical force, i.e. $\mathrm{I}\sim\mathrm{F}^2$, as consequence of the quantum degeneracy. We will collate our theoretical prediction with experimental AFM/STM measurements of single atom point contacts and complex DFT simulations to unambiguously prove the existence of these two characteristic regimes.

O 45: Metal Substrates II

Time: Wednesday 10:30–12:45 Location: H42

O 45.1 Wed 10:30 H42

Coadsorption of deuterium and CO on submonolayer Pt films on Ru(0001) model surfaces — Heinrich Hartmann, •Joachim Bansmann, Thomas Diemant, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Pt surfaces modified by Ru are of high interest for applications in low temperature Polymer Electrolyte (PE) fuel cells. Here, we report on a combined TPD/IRAS study of coadsorbed hydrogen (deuterium) and CO and their interaction with model surfaces, e.g., submonolayer Pt films on Ru(0001) with varying Pt coverages. The experimental results show that a closed CO layer completely blocks the adsorption of D_2. On a surface partly covered by CO, D_2 adsorption is still possible, however a considerable decrease of the D_{ad} adsorption energy is observed. In the reverse case, pre-adsorbed D_{ad} also reduces the amount of subsequently adsorbed CO, although CO adsorption is possible even on a closed D_{ad} layer. This phenomenon leads to very high total coverages (exceeding 1 ML) and an additional destabilization of the coadsorbed species. Pre-adsorbed D_{ad} has the strongest influence on the CO adsorption on Pt films with low Pt coverage (< 0.3 ML Pt). This trend can be explained by the considerably weaker D_{ad} binding energy on Pt islands compared to the Ru surface) which leads to a decreasing initial D_{ad} coverage and facilitates the displacement of D_{ad} by post-adsorbed CO. For the same reason the influence of pre-adsorbed CO on D_2 adsorption considerably increases with increasing Pt coverage, since D_{ad} is displaced to the less favorable Pt sites.

O 45.2 Wed 10:45 H42

Bimetallic PtAg/Pt(111) surfaces and their interaction with CO — •Thomas Diemant, Joachim Bansmann, and R. Jürgen

Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

The growth of Ag films on a Pt(111) substrate at room temperature and the formation of PtAg/Pt(111) surface alloys by annealing to higher temperature (up to 900 K) was studied by a combination of X-ray photoelectron spectroscopy (XPS) and temperature-programmed desorption (TPD) measurements. XPS measurements indicate a modification of the electronic properties of both components in the bimetallic surface layer; most prominently the binding energy of the Ag peaks shifts compared to pure Ag.

In the next step, the interaction of CO with structurally well-defined PtAg/Pt(111) surface alloys was studied by TPD and high resolution electron energy loss spectroscopy (HREELS). These alloys were formed by annealing to 900 K; their structural properties had already been clarified before by scanning tunnelling microscopy (STM) measurements in our institute. Both on the low as well as on the high temperature side of the platinum related CO TPD peak additional features arise after alloy formation. Furthermore, a peak related to CO adsorption on Ag sites is detected at 150 K in the CO TPD spectra.

O 45.3 Wed 11:00 H42

DFT-studies of interfacial processes in fluoride ion batteries — •Katrin Forster-Tonigold[1] and Axel Gross[1,2] — [1]Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, 89069 Ulm, Germany — [2]Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

Fluoride ion batteries (FIBs) are highly attractive systems for electrochemical energy storage as they offer substantially larger theoretical energy densities compared to conventional lithium ion batteries. The basic electrochemical reaction underlying FIBs is the conversion reaction: $m\mathrm{M} + n\mathrm{M}'\mathrm{F}_m \rightleftharpoons m\mathrm{MF}_n + n\mathrm{M}'$ with fluoride anions acting as charge transfer ions [1].

The performance of FIBs crucially depends on the fluoride ion transport through the electrolyte. As a possible route towards fluoride ion conducting, liquid electrolytes might be the use of shuttle molecules, that collect fluoride ions from the metal fluoride and release them at the metal. Therefore, molecules with a well-balanced fluoride binding energy are needed. Especially the first step of the conversion reaction, i.e. the adsorption and desorption of the shuttle molecule at the metal and metal fluoride substrate, could be crucial. To provide an insight into these initial processes occuring at the electrode-electrolyte interface of FIBs, we employ DFT calculations. We aim to find trends among different main group elements used in possible candidates for shuttle molecules. Besides, we try to understand the impact of various rest groups on the binding properties.

[1] M. A. Reddy and M. Fichtner, J. Mater. Chem. **21**, 17059 (2011).

O 45.4 Wed 11:15 H42

Kinetics of Single D_2O Molecules and Dimers on Cu(111) — •Cord Bertram and Karina Morgenstern — Lehrstuhl für Physikalische Chemie 1, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum

Water is well-known to form hydrogen-bonded networks on metal surfaces with a high structure variety, even at low temperature. Previous work on Cu(111) explored this variety by observing different amorphous and crystalline phases (Mehlhorn et al., Phys. Rev. Lett. 99 (2007), 246101). For further understanding of these networks, it is useful to analyse the kinetics of single molecules and the formation of nanoclusters. In this talk, we will discuss the diffusion of single D_2O molecules and dimers on Cu(111) measured by low temperature time-lapsed scanning tunneling microscopy. We deposit D_2O onto the surface below a temperature of 15 K with fluxes below $1.54\cdot10^{-4}\ \frac{\mathrm{molecules}}{\mathrm{nm}^2\mathrm{s}}$. The diffusion of monomers, the formation of dimers, and the subsequent diffusion of dimers is recorded between 19 K and 29 K. The height of the diffusion barrier and the prefactors are determined via the Arrhenius law. Surprisingly both species show similarities to the diffusion via tunneling of hydrogen. The results will be compared to previous works on e.g. Pd(111), Pt(111), and Ag(111) (Mitsui et al., Science 297 (2002) 1850; Motobayashi et al., Surf. Sci. 602 (2008) 3136).

O 45.5 Wed 11:30 H42

Study of Alloyed Gold Surfaces by Photon Emission STM — Birsen Kesik, Elif Peksu, Selman Tamer, Dilek Yildiz, and •Oğuzhan Gürlü — Istanbul Technical University, Department of Physics, Maslak, 34469, Istanbul, Turkey

Photon emission from surfaces, simultaneously with the surface topography measurements with Scanning Tunneling Microscopy was observed on various surface systems. Several types of photon detection mechanisms were developed. Regardless of the surfaces under consideration or the set up used, it is well known that the photon emission spectrum and intensity heavily depends on both the tip material and the tip geometry. We modified a commercial STM and implemented our photon collection setup; also a modified tip preparation procedure was employed. Using this setup we studied the photons emitted from different gold surfaces with various surface morphologies. Contrary to common knowledge, the intensity of the photon emission from similar regions of a rough Au surface was observed to be different. The local surface morphology was correlated to the photon emission intensity, as well as to the spectrum of the emitted photons. Here we suggest the possible dependence of the intensity and spectra of the emitted photons on the local alloying of the gold surfaces (Supported by TUBITAK 109T687).

O 45.6 Wed 11:45 H42

Surface structure of ultrathin Fe films on Ag(001) post-deposition annealed in O_2 atmosphere — •Daniel Bruns, Steffen Jentsch, Sören Lindemann, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

Iron oxides are used in different applications as spintronics or heterogeneous catalysis. In this work, ultrathin Fe films grown at room temperature on Ag(001) were post-deposition annealed in 10^{-5} mbar O_2 atmosphere at 300°C for 50 minutes. Since the surface has a strong influence on the properties of ultrathin films, the surface structure was investigated by Low Energy Electron Diffraction (LEED) and Scanning Tunneling Microscopy (STM). Submonolayer Fe films wet the Ag(001) substrate due to annealing in oxygen forming at least partial FeO, as concluded from LEED. Straight trenches aligned either in Ag[110] or Ag[$1\bar{1}0$] direction separate different FeO domains. On the other hand, with increasing Fe coverage the films show a three dimensional behavior upon annealing forming several exposed layers. In this case, LEED suggests two hexagonal structures as well as two low ordered rectangular structures rotated by 90° against each other, respectively. These structures were found to be located on different exposed layers at the surface via STM. The topmost layer of the oxidized films revealed a poorly ordered (2×3) superstructure, while the hexagonal surface structure was only found on deeper exposed layers. We created models to describe the observed surface structures suggesting partial formation of FeO as well as $Fe_3O_{4-\delta}$ at the surface.

O 45.7 Wed 12:00 H42

Kinetic vs. thermodynamic limitations of the formation of PtCu submonolayer alloys on Ru(0001) single crystals. — •Albert K. Engstfeld, Christoph K. Jung, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Core shell particles consisting of a metal A rich shell and a bi- or multialloy core, show a catalytic activity which may strongly differ from that of the pure metal particles. An interesting example are Pt enclosed alloy particles containing Cu, Co and Pt, which were found to be much more active to-wards O2 electroreduction than pure Pt. In this work we focus on the formation of Pt and Cu submonolayer alloys on Ru(0001), which represents the core for a core shell model catalyst. The surfaces have been investigated under ultra high vacuum conditions, using scanning tunneling microscopy (STM), to reveal the surface morphology as well as the atom distribution within the surface alloy. The limitation in the preparation of the surface alloy is the temperature, since at 750 K Pt starts intermixing with the Ru(0001) substrate. Just below this temperature, the intermixing of Cu and Pt on the surface is however kinetically hindered, which leads to coexistent mixed and unmixed 2D phases of both metals. Optimizing the experimental conditions (e.g. evaporation sequence, temperature ...), we are able to prepare short-range ordered monolayer surface alloys covering the entire surface over the full concentration regime (0-100%), The distribution of surface atoms in the monolayer surface alloys will be discussed based on the Warren Cowley short-range order parameters.

O 45.8 Wed 12:15 H42

The study of Pb self-diffusion from first principles — •Xiaohang Lin and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

With the single-atom transistor [1], the first actively switchable electronic device on the atomic scale was demonstrated. By the controlled relocation of one individual atom within an electrochemically fabricated metallic quantum point contact, an electrical current could be switched on and off. Changes in the atomic-scale structure within the contact area controlled by the electrode potential in an electrochemical set-up result in conductance changes of the atomic-scale contact.

Here, we study atomic-scale relocation processes in contacts form at Pb electrodes with periodic density functional theory (DFT) calculations. It is known that diffusion processes play a crucial role during the atomic-scale deposition and structure formation. For this reason, as a first step barriers for self-diffusion processes have been calculated using automatic transition state search routines. In order to address structured surfaces more realistically, an emphasis has been put on processes near step edges. It turned out that at such edges, two-particle exchange processes are very important for the diffusion in contrast to the "naive" direct single-particle hopping mechanism.

[1] F.-Q. Xie, L. Nittler, Ch. Obermair, Th. Schimmel, Phys. Rev. Lett. **93**, 128303 (2004).

O 45.9 Wed 12:30 H42

Mechanism of anisotropic crystal growth of gold nanorods — •Paul Erhart[1], Kasper Moth-Poulsen[1], and Mihail Popescu[2] — [1]Chalmers University of Technology, Gothenburg, Sweden — [2]University of South Australia, Adelaide

Anisotropic noble metal nanostructures are of general interest due to their optical and physical properties. Specifically, Au nanorods can be grown by immersing nanoparticles in supersaturated solution and addition of specific surfactants, which induce a strong anisotropy in the growth of (100) and (111) facets. While it is known that aspect ratio and quality of the final nanorods are affected by the choice of surfactant, a qualitative understanding of surface-surfactant interaction and growth mechanism are lacking.

In the present work we address these points by a combination of density functional theory (DFT) calculations and kinetic Monte Carlo (kMC) simulations. The most common surfactant is cetyl trimethyl ammonium bromide (CTAB), which interacts with the surface via a Br atom. This allows us to focus our attention on the behavior of Br on Au surfaces. We systematically determined adsorption and migration energies for both Br and Au adatoms and small clusters on flat (100) and (111) surfaces as well as surface steps. We find a strong asymmetry in the migration of both species between (100) and (111) surfaces. More importantly we identified a pathway for growth of (111) facets that does not require desorption of Br (or CTAB molecules). Using the DFT data we then parametrized a kMC model to study the dynamics of the growth process taking into account surface coverage and temperature.

O 46: Nanostructures and Clusters

Time: Wednesday 10:30–12:30 Location: H45

O 46.1 Wed 10:30 H45

$M\mathrm{Si}_n\mathrm{H}_n$ aggregates: from simple building blocks to highly magnetic functionalized materials — •Dennis Palagin and Karsten Reuter — TU München

The use of multi-doped endohedral Si clusters as building blocks for assembly at the nanometer scale has attracted much attention due to promising cage-like geometries and easy-to-tune electronic properties [1]. For instance, in these structures the high magnetic moments of transition metal dopants can be preserved through minimizing the cage-dopant interaction by hydrogen termination [2]. A variable amount of hydrogen atoms may be used to control the number of bonding sites of the cluster, to which another cage can be attached. With a tool box of monomers with differing numbers of "docking sites", it seems possible to build network architectures of any morphology. Here we scrutinize this proposition through density-functional theory based global geometry optimization. Our results show that, unlike in case of typical clathrate structures, $M\mathrm{Si}_{20}\mathrm{H}_{20}$ clusters tend to aggregate through the formation of double Si-Si "bridges" between the monomers. Intriguingly, such aggregates possess very high magnetic moments due to their virtually isolated dopants. We screen a larger range of possible oligomers and critically discuss the resulting geometrical and electronic structures.

[1] T. Iwasa and A. Nakajima, J. Phys. Chem. C 116, 14071 (2012).

[2] D. Palagin and K. Reuter, Phys. Rev. B 86, 045416 (2012).

O 46.2 Wed 10:45 H45

A full-dimensional and reactive neural network potential for water clusters based on first-principles — •Tobias Morawietz and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Artificial neural networks (NNs) provide an unbiased way to construct accurate interatomic potentials for a wide range of systems [1]. For this purpose a set of energies and forces obtained from electronic structure calculations is interpolated. The obtained NN potential can be evaluated several orders of magnitude faster than the underlying electronic structure data allowing to perform accurate simulations on extended length and time scales. Here, we report a full-dimensional NN potential for water clusters containing up to ten water molecules trained to density-functional theory (DFT) data [2,3]. Unlike other potentials for water based on first-principles, our potential is not constructed employing a truncated many-body expansion and is thus able to describe reactions involving proton transfer. Binding energies for global and local minima obtained with the NN potential typically deviate by less than 1 % from the DFT values.

[1] J. Behler, PCCP **13**, 17930 (2011).

[2] T. Morawietz, V. Sharma, and J. Behler, JCP **136**, 064103 (2012).

[3] T. Morawietz and J. Behler, submitted (2012).

O 46.3 Wed 11:00 H45

First-principles study of the interaction and charge transfer between gold clusters and TiO_2 nano-structures — •Chunsheng Liu, Ran Jia, Harald Oberhofer, and Karsten Reuter — TU München, Germany

Recent experimental studies of catalysis on small $(\mathrm{TiO}_2)_m$-Au_n hetero-clusters [J. Phys. Chem. A **115**, 11479 (2011)] have opened up a new direction in the search for efficient, yet stable (photo-)catalysts for reactions such as CO oxidation or water splitting. They have shown a strong dependence of the reactivity on the atomic stoichiometry of the catalyst clusters, including an especially pronounced even/odd behavior with respect to the number of Au atoms. In our contribution we discuss our findings - gained from *ab initio* global geometry optimization - leading to a theoretical understanding of the observed properties of nano-scale $(\mathrm{TiO}_2)_m$-Au_n hetero-clusters. Analogous to experiment, we find an even/odd behavior of the coated clusters' HOMO-LUMO gap and charge transfer from the coating Au atoms, which in turn influences the clusters' reactivities. Finally, we compare these properties of the $(\mathrm{TiO}_2)_m$-Au_n hetero-clusters to those of small gold Au_n particles adsorbed on extended TiO_2 surfaces, in order to gauge how much of the observed behavior is due to the limited size of the TiO_2 substrate cluster.

O 46.4 Wed 11:15 H45

Substrate-dependent dynamics of truly monodisperse Pd clusters under the STM — •Michael König[1], Bo Wang[1], Yves Fukamori[1], Bokwon Yoon[2], Friedrich Esch[1], Ueli Heiz[1], and Uzi Landman[2] — [1]Chemistry Department, Technische Universitat Munich, 85748 Garching, Germany — [2]School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, United States

We developed preparing truly monodisperse cluster-assembled materials via deposition of size-selected, soft-landed Pd clusters on epitaxial graphene to enable to fully complement STM with integral methods.

Our STM measurements show that the Pd clusters are well-dispersed on the graphene surface at room temperature (RT). Pd19/Pd20 clusters show both 2 and 3 monolayer high atomic structures, like clusters in the gas phase, but can be distinguished by slightly different height histograms. Neither cluster fragments, nor surface damage are observed, confirming a well-controlled soft-landing on the graphene surface [1].

The clusters on graphene/Ru(0001) are exclusively adsorbed on the ring-fcc registry of the superstructure, indicating a strong carbon-metal interaction and a softening of the carbon-carbon bonding at this local registry. The STM study reveals that the cluster mobility depends on the cluster footprint, e.g. Pd12 clusters show already at RT isomer-dependent diffusion [1]. Finally, the substrate and temperature dependent ripening processes were examined via variable temperature STM. [1]B. Wang, B. Yoon, M. Konig, Y. Fukamori, F. Esch, U.Heiz and U. Landman, Nanoletters 12, 5907 (2012)

O 46.5 Wed 11:30 H45

A key to understanding gold nanoalloys: the interplay of fluxionality and electronic structure — •Linn Leppert[1], Rodrigo Q. Albuquerque[2], Adam S. Foster[3], and Stephan Kümmel[1] — [1]Theoretische Physik IV, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Institute of Chemistry of São Carlos, University of São Paulo, 13560-970 São Carlos-SP, Brazil — [3]Department of Applied Physics, Aalto University School of Science, P.O. Box 11100, FI-00076 Aalto, Finland

The high catalytic activity of Au nanoparticles (NP) is a prime example for the special properties of metal clusters. By alloying, e.g. with Pt, the properties of Au NP can further be significantly improved. Turnover rates in methanol fuel cells and other oxidation reactions are practically relevant examples. However, the fundamental question of why alloying improves the NP properties is still poorly understood. The finding that the high catalytic activity of Au-Pt nanoalloys is observed in a variety of reactions indicates that there is a combination of rather fundamental, basic properties that are not specific to certain chemical environments and that can be optimized by alloying. We show that electronic properties that are relevant for chemical reactivity, e.g. the density of states (DOS) at the Fermi level and the spatial orbital structure, can be associated with Pt. On the other hand we demonstrate that an increasing amount of Au increases the Au-Pt NP fluxionality. Thus, by combining Au and Pt both the DOS and the particle's fluxionality can be adjusted and a catalytically optimal interaction strength between catalyst and reactants be obtained.

O 46.6 Wed 11:45 H45

Mass selected copper and silver clusters on rare gas layers: Photoelectron spectroscopy with ultraviolet light — •Christoph Schröder[1], Natalie Miroslawski[1], Paul Salmen[1], Bernd von Issendorff[2], and Heinz Hövel[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Fakultät für Physik, Universität Freiburg, 79104 Freiburg, Germany

Mass selected Cu_N and Ag_N clusters, with N=55,92,147 were soft landed at T=15K-25K on different substrates covered with rare gas layers. Up to 9 spots, with different cluster size and coverage, could be deposited on one and the same sample for better comparability. These spots were investigated by ultraviolet photoelectron spectroscopy using 11.6 eV photon energy in ultrahigh vacuum (UHV). In order to cut off the satellite of the ultraviolet light and achieving an UHV below 10^{-10} mbar we used a LiF window [1]. Caused by the low photon energy we obtained a size dependent cluster signal for energies in the s-p-band region which are discussed in respect of free beam experiments [2].

[1] M.Budke and M.Donath, Appl. Phys. Lett. **92**, 231918 (2008); S.Suga et al., Rev. Sci. Instruments **81**, 105111 (2010)
[2] Oleg Kostko, *Photoelectron spectroscopy of mass-selected sodium, coinage metal and divalent metal cluster anions.* PhD-thesis, Albert-Ludwig-Universität Freiburg (2007)

O 46.7 Wed 12:00 H45

The effect of oxygen on the morphology of Au nanoparticles — •Darius Pohl[1,2], Alexander Surrey[1,2], Ludwig Schultz[1,2], and Bernd Rellinghaus[1] — [1]IFW Dresden, P.O. Box 260116, D-01171 Dresden, Germany. — [2]TU Dresden, Institute for Solid State Physics, Dresden, Germany.

We present an easy procedure for the synthesis of single crystalline gold nanoparticles with a mean diameter of 4 nm by using a DC-sputtering in an argon-oxygen gas mixture. Morphology population statistics for a large amount of particles have been determined to quantify the influence of oxygen. It is found that the particles undergo a structural transition from predominantly icosahedral to single crystalline particles with increasing amount of oxygen. Aberration-corrected HRTEM investigations prove that likewise prepared single crystalline nanoparticles are defect and oxygen free. In contrast, icosahedral particles prepared in pure argon atmosphere reveal the presence of edge dislocations pointing to an energetic disfavoring already at these relatively small particle sizes. The impact of oxygen on the early growth process of Au nanoparticles will be discussed in detail.

O 46.8 Wed 12:15 H45

XANES measurements on Ag clusters deposited in silica aerogel and ionic liquid — •David Engemann[1], Sabrina Hoffmann[1], Stefanie Duffe[1], Christian Sternemann[1], Kristina Kvashnina[2], Pieter Glatzel[2], Ralph Wagner[3], and Heinz Hövel[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund — [2]ESRF, Grenoble, France — [3]BU Wuppertal, Fachgruppe Physik-Materialwissenschaften, Wuppertal

Properties of clusters, in this case silver clusters, can differ widely from that of the corresponding bulk material. These differences correspond to the size of the clusters, their chemical environment and, in the case of deposited clusters, the supporting material. For most applications and measurements on deposited clusters it is necessary to deposit high amounts of clusters while protecting them from coalescence.

Silica aerogel is a very porous network (up to 99% empty space) of SiO_2 nanoparticles with interparticle distances of about 50 nm. Depositing clusters (high amounts up to several cluster monolayers) in the nano-porous surface can prevent them from coalescence.

Clusters deposited in these matrices are still in contact to the gases in their surroundings. Chemical reactions like sulfidizing were investigated with plasmon resonance measurements and X-ray Absorption Near Edge Structure spectroscopy (XANES).

Further experiments with Ag clusters deposited in Room Temperature Ionic Liquids (RTIL) are in progress.

O 47: Gaede Prize Talk – Kirsten von Bergmann

Time: Wednesday 13:15–13:55 Location: H15

Prize Talk O 47.1 Wed 13:15 H15

Complex magnetic order on the atomic scale — •Kirsten von Bergmann — Institute of Applied Physics, University of Hamburg

Magnetism in low-dimensions is a versatile topic and broken inversion symmetry due to the presence of a surface can induce the formation of complex magnetic order. Here the driving force for the canting of adjacent magnetic moments is the spin-orbit induced Dzyaloshinskii-Moriya interaction. Thin magnetic films on heavy substrates are good candidates for this kind of surface-induced non-collinear magnetic states with unique rotational sense.

Spin-polarized scanning tunneling microscopy (SP-STM) combines magnetic sensitivity with high lateral resolution and therefore grants access to such complex magnetic order with unit cells on the nanometer scale. Several non-collinear magnetic ground states, such as spin spirals where the spin rotates from one atom to the next, habe been observed [1-3]; while in uniaxial systems only one propagation direction is found, in biaxial systems rotational domains of spin spirals are present. In the case of the monolayer Fe on Ir(111) a combination of different magnetic interactions, including higher-order interactions, leads to a two-dimensional lattice of magnetic skyrmions on the atomic scale [4,5].

[1] M. Bode et al., Nature 447, 190 (2007).
[2] P. Ferriani et al., Phys. Rev. Lett. 101, 27201 (2008).
[3] M. Menzel et al., Phys. Rev. Lett. 108, 197204 (2012).
[4] K. von Bergmann et al., Phys. Rev. Lett. 96, 167203 (2006).
[5] S. Heinze et al., Nature Phys. 7, 713 (2011).

O 48: Invited Talk (Florian Klappenberger)

Time: Wednesday 15:00–15:45 Location: H36

Invited Talk O 48.1 Wed 15:00 H36

Surface-confined molecular nanoarchitectures: non-covalent and covalent construction and templated dynamics — •Florian Klappenberger — Physik Department E20, James-Franck-Str.1, 85748 Graching

The in vacuo engineering of molecular nanoarchitectures using non-covalent interactions and covalent bonding between carefully designed building blocks on well-defined surfaces is investigated with a complementary multitechnique approach combining scanning tunneling microscopy and X-ray spectroscopy with the appropriate theoretic tools. First, the hierarchic formation principles of supramolecular networks combining hydrogen bridges, proton acceptor ring interactions and metal-organic bonding are unraveled and some exemplary functionalities, e.g., the confinement of electrons or the controlling of the growth of magnetic clusters, are reviewed. In addition, the nanoporous architectures can control translational, rotational and constitutional dynamics and provide a new way to study such phenomena on the single molecule level. We present a detailed analysis of the caged molecular dynamics by molecular force-field simulations customized on the basis of density functional theory calculations. In the second part, the construction of novel carbon scaffolds with the help of an on-surface covalent reaction formally reminiscent of the Glaser-Hay homo-coupling of terminal alkynes is discussed. After showing the controlled formation of dimerized species and polymerized irregular networks we discuss our current understanding of the reaction pathway on the noble metal Ag(111) surface differing from the classic pathway on more reactive substrates.

O 49: Symposium Quantum Plasmonics (SYQP, jointly with HL, TT)

Time: Wednesday 15:00–18:05 Location: H1

Invited Talk O 49.1 Wed 15:00 H1

Quantum plasmonics and applications in light harvesting — •Peter Nordlander — Department of Physics, Rice University, Houston TX 77251, USA

Quantum effects can have a pronounced influence on the on the optical properties of strongly coupled nanoparticles.[1] For closely spaced metallic nanoparticles, electron transfer and nonlocal screening can drastically reduce the electric field enhancements across the gap and result in a Charge Transfer Plasmon (CTP) where an oscillatory electric tunneling current flows between the particles,[2] and strongly nonlinear effects can be induced.[3] The energy of the CTP is found to depend strongly on the electronic structure of the junction and the presence of molecules inside the gap.[4] For the coupled plasmonic-excitonic system where hybrid plexciton states are formed,[5] quantum effects can strongly modify the optical spectrum and a induce highly nonlinear optical response. Another plasmonic quantum mechanical effect is the nonradiative decay of plasmons into hot electron-hole pairs which can induce chemical reactions on the surface of the nanostructure [6] or be harvested directly in photodetector or photovoltaic geometries.[7]

References [1] J. Zuloaga et al., ACS Nano 4(2010)5269 [2] R. Esteban et al., Nat. Comm. 3(2012)825 [3] C. Marinica et al., Nano Lett. 12(2012)1333 [4] P. Song et al., Phys. Rev. B 86(2012)121410 [5] A. Manjavacas et al., Nano Lett. 11(2011)2318; ACS Nano 6(2012)1724 [6] S. Mukherjee et al., Nano Lett. 13(2013)nl303940z [7] M. W. Knight et al., Science 332(2011)702; Z.Y. Fang et al., Nano Lett. 12(2012)3808

Invited Talk O 49.2 Wed 15:30 H1

Deterministic quantum plasmonics with single nanodiamonds — •Serge Huant[1], Oriane Mollet[1], Aurelien Cuche[1,2], and Aurelien Drezet[1] — [1]Institut Neel, CNRS and Univ. Joseph Fourier, BP 166, 38042 Grenoble, France — [2]CEMES, CNRS, BP 94347, 31055 Toulouse, France

Using an all-optical scheme, we can attach a single nanodiamond (ND) hosting a few nitrogen-vacancy (NV) color centers onto fiber tips for near-field scanning optical microscopy (NSOM). Illuminating the grafted ND with the substrate fiber and using the fluorescence generated by the ND as source of light achieves a genuine quantum scanning optical microscopy that operates at room temperature thanks to the exceptional photostability of the NVs. In addition, we have found that the ND-based active tip is capable of launching surface-plasmon-polaritons (SPPs) into gold films. Since the ND is a quantum source of light, a limited number of single plasmons are created, depending on the actual NV occupancy. A critical prerequisite for using these SPPs in future quantum protocols is that their propagation does not destroy their quantum coherence.

In this talk, we will review our demonstration of quantum SPP launching with a ND-based active tip. Then we will demonstrate that the quantum character of the light emanating from the ND is preserved by the plasmon mediation along the gold film. Our findings open the way to a deterministic quantum plasmonics, where a well-controlled number of quantum SPPs is launched at any freely chosen position in a plasmonic receptacle.

Invited Talk O 49.3 Wed 16:00 H1

Optically-active hybrid nanostructures: Exciton-plasmon interaction, Fano effect, and plasmonic chirality — •Alexander Govorov — Ohio University, Athens, OH, USA

Excitons and plasmons in nanocrystals strongly interact via Coulomb and electromagnetic fields and this interaction leads to characteristic interference effects which can be observed in optical spectra. An interaction between a discrete state of exciton and a continuum of plasmonic states gives rise to Fano-like asymmetric resonances and anti-resonances [1,2]. These interference effects can strongly enhance visibility of relatively weak exciton signals and can be used for spectroscopy of single nanoparticles and molecules. If a system includes chiral elements (chiral molecules or nanocrystals), the exciton-plasmon interaction is able to alter and enhance circular dichroism (CD) of chiral components [3,4]. Recent experiments on molecule-nanocrystal and multi-nanocrystal complexes have confirmed our predictions [4]. Potential applications of dynamic hybrid nanostructures include sensors and new optical and plasmonic materials.

1. W. Zhang, G. W. Bryant, A. O. Govorov, Phys. Rev. Lett. 97, 146804 (2006). 2. M. Kroner, A. O. Govorov, S. Remi, B. Biedermann, S. Seidl, A. Badolato, P. M. Petroff, W. Zhang, R. Barbour, B. D. Gerardot, R. J. Warburton, and K. Karrai, Nature 451, 311 (2008). 3. A.O. Govorov, Z. Fan, P. Hernandez, J.M. Slocik, R.R. Naik, Nano Letters 10, 1374 (2010). 4. A. Kuzyk, R. Schreiber, Z. Fan, G. Pardatscher, E.-M. Roller, A. Högele, F.C. Simmel, A. O. Govorov, T. Liedl, Nature, 483, 311 (2012).

Coffee break

Invited Talk O 49.4 Wed 17:00 H1

Quantum nano-optics: Interaction of metallic nano-particles with quantum emitters — •Salvatore Savasta — Università di Messina, I-98166 Messina, Italy

Metallic nanoparticles and nanostructures are able to focus the electromagnetic field on sizes considerably smaller than a wavelength. This ability is due to the existence of collective electronic excitations on the surface of metal particles called plasmons. In this way, it is possible to increase the optical density of states as well as with the microcavities but with much more compact structures [1].

We discuss the quantum optical properties of hybrid artificial molecules composed of an individual quantum emitter and a metallic nanoparticle. The coupling between the two systems can give rise to a Fano interference effect which strongly influences the quantum statistical properties of the scattered photons [2]. Laser cooling the center-of-mass motion of nano-systems that exhibit Fano resonances is also discussed[3].

We also show, by accurate scattering calculations, that a system constituted by a single quantum emitter placed in the gap between two metallic nanoparticles [4]. Metallic-nanoparticles coupled to many quantum emitters can also achieve the ultrastrong coupling regime [5].

[1] S. A. Maier, Plasmonics: Fundamentals and Applications (Springer, New York, 2007). [2] A. Ridolfo *et al.*, Phys. Rev. Lett. **105**, 263601 (2010). [3] A. Ridolfo *et al.*, Phys, Rev, Lett. **106**, 013601 (2011). [4] S. Savasta *et al.*, ACS Nano **4**, 6369 (2010). [5] A. Ridolfo *et al.*, **109**, 193602 (2012).

Invited Talk O 49.5 Wed 17:30 H1

Non-dipolar & magnetic interactions with optical antennas — Alberto Curto[1], Martin Kuttge[1], Marta Castro-López[1], Ion Hancu[1], Tim Taminiau[2], and •Niek van Hulst[1,3] — [1]ICFO - The Institute of Photonic Sciences, Castelldefels, Barcelona — [2]Kavli Institute of Nanoscience Delft, the Netherlands — [3]ICREA - Barcelona

Plasmonic antennas are ideal to manage the interaction with single photon emitters, such as quantum dots or fluorescent molecules [1]. Tailoring the electromagnetic mode one can control electronic transitions rates and angular emission patterns, which is key for bright directed single photon sources [2]. Here we present three different examples of hybrid emitter-antenna coupled systems where electric dipole, quadrupole or magnetic dipole moments are dominant. Experimental angular radiation patterns show striking differences in the emission of resonant and non-resonant magnetic modes excited by local light sources [3]. Finally we present a magneto-electric antenna: by exploiting the interference between magnetic and electric modes we experimentally realize a compact and robust optical antenna for directed photon emission, which outperforms larger, multi-element antennas in both bandwidth and directionality.

[1] AG Curto et al. Unidirectional emission of a Q-dot coupled to a nanoantenna, Science 329, 930 (2010)

[2] TH Taminiau et al. Optical nanorod antennas as cavities for dipolar emitters: sub- & super-radiant modes, NanoLett. 11, 1020 (2011)

[3] AG Curto et al. Magnetic Resonance of a Nanoslot Optical Antenna, Submitted

Concluding remarks

O 50: Focussed Session: Majorana Fermions in Condensed Matter (jointly with DS, HL, MA, and TT)

Majorana fermions arise as quasi-particle excitations in condensed matter systems which exhibit non-Abelian exchange statistics. This property makes them a fundamentally new type of particles, and possibly allows topological quantum computing in this system. In the last few years, the study of Majorana fermions has rapidly evolved from being a mere theoretical concept to a practical realization: Following theoretical proposals involving hybrid nanosystems consisting of conventional superconductors and semiconducting nanowires, experiments have now found signatures of Majorana fermions. This Focused Session will discuss various aspects of Majorana fermions and the hybrid systems hosting them, including both theoretical and experimental contributions.

Organizers: Fabian Hassler (RWTH Aachen), Michael Wimmer (Leiden University)

Time: Wednesday 15:00–18:00 Location: H20

Invited Talk O 50.1 Wed 15:00 H20

Subgap States in Majorana Wires — •Piet Brouwer — Freie Universität Berlin

A one-dimensional spin-orbit coupled nanowire with proximity-induced pairing from a nearby s-wave superconductor may be in a topological nontrivial state, in which it has a zero energy Majorana bound state at each end. In this talk, I will discuss how non-idealities in this proposal, such as potential disorder, deviations from a strict one-dimensional limit, or details concerning the termination of the wire, affect the topological phase and its signatures in a current-voltage measurement. In particular, I'll argue that the topological phase can persist at weak disorder or for multichannel wires, although some of the signatures of the presence of Majorana fermions are obscured.

Invited Talk O 50.2 Wed 15:30 H20

New Measurements on Nanowire Majorana Systems — •Charles Marcus[1,3], Hugh Churchill[2,3], Mintang Deng[4], and Hongqi Xu[4] — [1]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Copenhagen, DK — [2]Department of Physics, MIT, Cambridge, MA USA — [3]Department of Physics, Harvard University, Cambridge, MA USA — [4]Division of Solid State Physics, Lund University, Lund, Sweden

This talk will present recent measurements on gated InSb nanowires coupled to a superconducting film. This set-up is one designed to detect Majorana end states. We show data similar to that seen in other groups recently, and also extend measurements in a number of directions, including higher field and higher conductance. Oscillatory structure suggesting interacting end-state Majoranas is found. We also identify transport regimes where even-odd Kondo-like features are evident, combined with Andreev bound states.

This research is sponsored by Microsoft Project Q, the Danish National Research Foundation, and Harvard University.

Topical Talk O 50.3 Wed 16:00 H20

Adaptive Tuning of Majorana Fermions in a Quantum Dot Chain — •Anton Akhmerov — Harvard University, USA

I will explain how to overcome the obstacles that disorder and high density of states pose to the creation of unpaired Majorana fermions in one-dimensional systems. This is achieved by splitting the system into a chain of quantum dots, which are then tuned such that the chain can be viewed as an effective Kitaev chain with maximally localized Majorana fermions. Resonant Andreev spectroscopy allows us to make this tuning adaptive, so that each pair of dots may be tuned independently of the other. Our numerical simulations show that already in three quantum dots it is possible to have almost completely decoupled Majorana fermions.

15 min. break

Topical Talk O 50.4 Wed 16:45 H20

Majorana Fermions in Disordered Quantum Wires — •Alexander Altland — Institute for Theoretical Physics, Zülpicher Str. 77, 50937 Köln

Proximity coupled spin-orbit quantum wires have recently been shown to support midgap Majorana states at critical points. We show that in the presence of disorder these systems are prone to the buildup of a second bandcenter anomaly, which is of different physical origin but shares key characteristics with the Majorana state: it is narrow in width, insensitive to magnetic fields, carries unit spectral weight, and is rigidly tied to the band center. Depending on the parity of the number of subgap quasiparticle states, a Majorana mode does or does not coexist with the impurity generated peak. The strong 'entanglement' between the two phenomena may hinder an unambiguous detection of the Majorana by spectroscopic techniques.

Topical Talk O 50.5 Wed 17:15 H20

Parity Effects and Crossed Andreev Noise in Transport through Majorana Wires — •Bernd Rosenow[1], Björn Zocher[1,2], and Mats Horsdal[1] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04009 Leipzig, Germany — [2]Max-Planck-Institute for Mathematics in the Sciences, D-04103 Leipzig, Germany

One of the defining properties of a topologically ordered state is the ground state degeneracy on surfaces with nonzero genus. In semiconductor-superconductor hybrid structures, a phase transition between regular and topologically nontrivial superconductivity is expected as a function of chemical potential or magnetic field strength. The difference in ground state degeneracies of the two phases is reflected in the parity and magnetic flux dependence of nonlinear Coulomb blockade transport through a ring shaped structure.

In nanowires of finite length, topologically non-trivial superconductivity is expected to give rise to Majorana bound states at the ends of the wire. The non-locality of Majorana bound states opens the possibility of crossed Andreev reflection with nonlocal shot noise, due to the injection of an electron into one end of the superconductor followed by the emission of a hole at the other end. When coupling the end states to leads via quantum dots with resonant levels, in the space of energies of the two resonant quantum dot levels we find a four peaked clover-like pattern for the strength of noise due to crossed Andreev reflection, distinct from the single ellipsoidal peak found in the absence of Majorana bound states.

O 50.6 Wed 17:45 H20

Majorana qubit rotations in microwave cavities — •Thomas L. Schmidt, Andreas Nunnenkamp, and Christoph Bruder — Department of Physics, University of Basel, CH-4056 Basel, Switzerland

Majorana bound states have been proposed as building blocks for qubits on which certain operations can be performed in a topologically protected way using braiding. However, the set of these protected operations is not sufficient to realize universal quantum computing. We show that the electric field in a microwave cavity can induce Rabi oscillations between adjacent Majorana bound states. These oscillations can be used to implement an additional single-qubit gate. Supplemented with one braiding operation, this gate allows to perform arbitrary single-qubit operations.

O 51: Focussed Session: Frontiers of Electronic Structure Theory V (jointly with HL and TT)

Time: Wednesday 16:00–19:30 Location: H36

Topical Talk O 51.1 Wed 16:00 H36

Screening high throughput density functional theory calculations using simplified models. — •Georg K. H. Madsen, Ingo Opahle, Alessandro Parma, Eunan J. McEniry, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, Bochum, Germany

Thermoelectric materials can be utilized for an efficient conversion of waste heat to electric power. Thermoelectric properties of known compounds can be rationalized and predicted using only the structure as an input.[1] While this can used to discover potential thermoelectric materials by screening known structures[2], there remains a large challenge in discovering unknown phases computationally. Employing a newly developed high throughput environment we show how the stability of binary transition metal silicides can be reproduced using a systematic replacement technique.[3]

As ternary and higher compounds are considered, a combinatorial explosion of potential structures and combinations must be considered. We have therefore develop ed tight binding models of the electronic structure and datamining methods based on the calculation of binary compounds. It will be discussed how these simplified models can be interpreted and used to pre-screen the stability of higher compounds to limit the number of density functional calculations to be done.

O 51.2 Wed 16:30 H36

Tight-binding scale-bridging calculations for steel research — •Nicholas Hatcher, Georg K H Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum, Germany

Parameterized methods to extend electronic structure calculations to large systems have recently garnered additional attention due to the limits of traditional DFT. The ability to model low carbon content in steel requires the accurate calculation of millions of atoms. However, interatomic potentials have been shown to be inconsistent with DFT in different environments and cannot give an accurate portrayal of chemical bonding or magnetism. Thus, a coherent transferable tight-binding (TB) parameterization was developed for Fe-C by extracting bonding interactions from DFT and finding a suitable interatomic repulsion. This model gives an accurate description of the energy hierarchy of relevant Fe-C structures, elastic properties, and defect energies. We apply this model to determine mechanisms of carbon segregation to grain boundaries and carbon diffusion in iron, including the interaction of multiple defects under tension and pressure. Furthermore, this intuitive energy functional forms the basis for bond order potentials, thereby extending system sizes to millions of atoms.

O 51.3 Wed 16:45 H36

Local atomic energies from optimal atomic orbitals — •Björn Lange, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

Decomposing the energy of a condensed matter system into atomic contributions is of great use e.g. for understanding the physical origin of defect and surface energetics or for identifying chemically reactive regions in disordered systems. However, commonly employed energy calculations in the framework of density-functional theory (DFT) do not in general provide a natural decomposition into atoms. Here we propose a novel scheme to achieve this based on the recently introduced concept of atom-centered Quamols[1] that are variationally optimized to represent the electronic structure with a minimal basis set, which largely avoids local overcompleteness issues. The spillage resulting from the remaining small incompleteness is segmented according to a space separation derived from the Quamol atomic densities, maintaining the accuracy of the underlying DFT calculation. The total energy is then decomposed by combining this basis set with a local energy density treatment based on the ideas of Chetty and Martin[2]. We demonstrate the performance of our scheme by visualizing and analyzing the energy distribution at surfaces and in amorphous silicon.

[1] PRB 84, 085101, (2011)
[2] Chetty, N. and Martin, Richard M., PRB 45, 6074, (1992)

O 51.4 Wed 17:00 H36

Environmental linear-scaling tight-binding for multicomponent metallic alloys — •Eunan J. McEniry, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany.

The development of accurate and transferable models to describe the behaviour of multicomponent systems is attracting considerable interest in materials modelling. Tight-binding models derived from density functional theory potentially provide an accurate and systematic approach to this problem. We introduce a methodology for environmental tight-binding (ETB) in which both the overlap and environmental contributions to the electronic structure are included. In order to implement the resulting ETB models within linear-scaling tight-binding approaches, a method for the evaluation of the screening matrix has been developed, based on a Chebyshev expansion of the inverse of the overlap matrix. The resultant linear-scaling environmental tight-binding framework has been applied to a number of relevant material systems, and the transferability and scalability of the approach is discussed. The present contribution outlines our attempts to extend the tight-binding approach towards larger-scale molecular dynamics simulations within a linear-scaling framework.

O 51.5 Wed 17:15 H36

Spontaneous Electric Polarisation from a Classical Perspective. — •Paul Tangney — Imperial College London, London, UK

Spontaneous polarisation is a quantity attributed to noncentrosymmetric crystals and is often associated with a macroscopic electric field permeating the bulk of a sample. Its time derivative is measured as a current density during application of an external stimulus, such as temperature, strain, or an electric field. I will argue that such currents do not require the existence of a spontaneous polarisation field or a macroscopic electric field in the bulk of a polar material. They can be explained by symmetry arguments within a purely classical picture and should be calculable from the time dependence of the many-particle position probability density function of the material's constituent charges - a classical quantity. The only macroscopic electric field across any bulk crystal arises from the charges on its surfaces, which in most cases are strongly influenced by surface relaxation/reconstruction and chemical environment and unlikely to be determined by polarization currents. I will show how the classical picture of polarisation presented is consistent with the Modern Theory of Polarisation[1], in all but interpretation. I will illustrate my arguments with simulations of a toy system.

[1] R. Resta and D. Vanderbilt, "Theory of Polarization: A Modern Approach", in Physics of Ferroelectrics: a Modern Perspective C.H. Ahn, K.M. Rabe, and J.M. Triscone, Eds. Springer-Verlag, (2007).

O 51.6 Wed 17:30 H36

Potential energy surface of $BaTiO_3$ explored with density-functional theory and classical force fields — •Joseph Fallon[1], David McComb[2], Arash Mostofi[1], and Paul Tangney[1] — [1]Imperial College London, London, UK — [2]The Ohio State University, Columbus, USA

Much is known about the electronic structure of $BaTiO_3$, its phonon dispersions, and the energetics of its long wavelength lattice distortions. However, there is much more to learn about the potential energy surface (PES) on which the atoms move. We study the PES using a combination of density functional-theory (DFT) and a polarisable ionic model of interatomic bonding. Our force field is in close agreement with DFT on structures, the PES, and phonon frequencies and allows accurate large scale atomistic simulations of domain structures and dynamics to be performed. A key advantage of an atomistic model over the coarse grained models that are often used to simulate domain dynamics is that it allows the simulation of heterogeneous materials (e.g. grain boundaries, point defects). However, we also point out some features of the PES, which may be important to domain dynamics, that effective Hamiltonians based on the transverse optic soft mode eigenvector and the local strain fail to capture.

O 51.7 Wed 17:45 H36

Efficient Oscillator-Based Approach for Polarizability and van der Waals Interactions — •Vivekanand Gobre[1], Robert A. Distasio Jr.[2], Roberto Car[2], Matthias Scheffler[1], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG — [2]Princeton University, USA

The dynamic polarizability measures the response to an applied time-dependent electric field, and its accurate determination is crucial for van der Waals (vdW) interactions and other response properties. First-principles calculations of polarizabilities in principle require a computationally expensive explicit treatment of many-electron excitations, and are only applicable in practice to systems with less than about 100 atoms. In this work, we present an efficient parameter-free approach for calculating accurate frequency dependent polarizabilities for molecules with thousands of atoms, as well as periodic materials. This is achieved by the synergistic coupling of the Tkatchenko-Scheffler method [1], which accurately treats short-range hybridization effects, with the self-consistent screening equation from classical electrodynamics [2,3]. Using only the electron density and free atom reference, we obtain an accuracy of 7% for both static polarizabilities and vdW coefficients for an extensive database of gas-phase molecules and crystals. We analyze the interplay of hybridization and long-range screening effects on the polarizability. [1] Tkatchenko and Scheffler, PRL (2009), [2] Felderhof, Physica (1974), [3] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012).

O 51.8 Wed 18:00 H36

Van der Waals interactions in Density Functional Theory and Linear-scaling Density Functional Theory — •Lampros Andrinopoulos, Nicholas D. M. Hine, and Arash A. Mostofi — Imperial College London, London, United Kingdom

Semilocal functionals in Density Functional Theory (DFT) achieve high accuracy simulating a wide range of systems, but miss the effect of dispersion (vdW) interactions, important in weakly bound systems. We study two different methods to include vdW in DFT: First, we investigate a recent approach [1] to evaluate the vdW contribution to the total energy using maximally-localized Wannier functions. Using a set of simple dimers, we show that it has a number of shortcomings that hamper its predictive power; we then develop and implement a series of improvements [2] and obtain binding energies and equilibrium geometries in closer agreement to quantum-chemical coupled-cluster calculations. Second, we implement the vdW-DF functional [3], using Soler's method [4], within ONETEP [5], a linear-scaling DFT code, and apply it to a range of systems. This method within a linear-scaling DFT code allows the simulation of weakly bound systems of larger scale, such as organic/inorganic interfaces, biological systems and implicit solvation models. [1] P. Silvestrelli, J.P.C. A 113, 5224 (2009). [2] L. Andrinopoulos et al, J.C.P. 135, 154105 (2011). [3] M. Dion et al, P.R.L. 92, 246401 (2004). [4] G. Roman-Perez, J.M. Soler, P.R.L. 103, 096102 (2009). [5] C. Skylaris et al, J.C.P. 122, 084119 (2005).

O 51.9 Wed 18:15 H36

Microscopic van der Waals Interactions with Localized and Metallic States — •Victor Gonzalo Ruiz, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG

Several promising methods have been developed in recent years for an efficient modeling of van der Waals (vdW) interactions in molecules and solids. However, essentially all of these methods rely on an localized model for the polarizability, ignoring the rather strong interplay between localized and metallic electronic states. Such states are present in many relevant materials, including transition metals, hybrid organic/metal interfaces, and topological insulators. Here we show how to extend the Tkatchenko-Scheffler method [1] for vdW interactions to treat localized and itinerant electronic states on equal footing by using the gradient of the electron density. In our model, the vdW correction vanishes for the homogeneous electron gas as it should in density-functional theory built upon the local-density approximation. To illustrate the performance of the newly developed microscopic model, we study the cohesive properties of coinage metals and the binding of organic molecules on metals. [1] A. Tkatchenko and M. Scheffler, PRL 102, 073005 (2009).

O 51.10 Wed 18:30 H36

Self-Consistent Density Functional Including Long-Range van der Waals Interactions — •Nicola Ferri[1], Robert A. Distasio Jr.[2], Roberto Car[2], Matthias Scheffler[1], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Princeton University, USA

Van der Waals (vdW) interactions are significant for a wide variety of systems, from noble-gas dimers to complex organic/inorganic interfaces. The long-range vdW energy is a tiny fraction ($\sim$0.001%) of the total energy, hence it is typically assumed that vdW interactions do not change electronic properties. Although the vdW-DF functional self-consistently includes the effect of the vdW energy on electronic structure [1], the influence of "true" long-range vdW interactions is difficult to assess since a significant part of vdW-DF energy arises from short distances. Here, we present a self-consistent implementation of the long-range Tkatchenko-Scheffler (TS) density functional [2], including its extension to surfaces [3]. The analysis of self-consistency for rare-gas dimers allows us to reconcile two different views on vdW interactions: (i) Feynman's view that advocates changes in the electron density, and (ii) atoms separated by an infinite barrier. In agreement with previous work [1], we find the contribution from self-consistency to be negligible in the structure and stability of vdW-bound complexes. However, a closer look at complex organic/inorganic interfaces reveals notable modification of the energy levels when using the self-consistent TS vdW density functional. [1] Thonhauser *et al.*, PRB (2007), [2] Tkatchenko and Scheffler, PRL (2009), [3] Ruiz *et al.*, PRL (2012).

O 51.11 Wed 18:45 H36

Many-Body van der Waals Interactions from Isotropically Damped Coupled Quantum Harmonic Oscillators — •Alberto Ambrosetti[1], Robert A. DiStasio Jr.[2], and Alexandre Tkatchenko[1] — [1]Fritz-Haber institut der MPG, Faradayweg 4-6 14195 Berlin, Germany — [2]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA

The current interest in functional materials with increasing size and complexity demands high accuracy in first-principles calculations. In these systems, the collective many-body (MB) description of van der Waals (vdW) interactions is indispensable to reach the highly coveted "chemical accuracy". The recently introduced DFT+MBD method (PRL **108**, 236402 (2012); PNAS **109** 14791 (2012)) for the dispersion energy based on a coupled set of quantum harmonic oscillators (QHOs) was shown to reach chemical accuracy for gas-phase molecules and molecular solids. Its formulation, however, makes the derivation of interatomic forces and a fully self-consistent DFT+MBD implementation non-trivial. We propose here a simplified approach, making use of a set of QHOs with isotropically damped dipole–dipole coupling, which provides an effective random-phase approximation treatment of their vdW interaction (arXiv:1210.8343). This allows for a simple analytical treatment of interatomic forces, yet providing high efficiency and accuracy. Application over a wide range of systems shows a consistent improvement with respect to pairwise approximations, particularly for the most extended systems.

O 51.12 Wed 19:00 H36

Interplay between H bond symmetrization and spin transition in ϵ-FeOOH: insights from first principles — •Carmen Quiroga and Rossitza Pentcheva — Dept. of Earth and Environmental Sciences, University of Munich

Structural and electronic spin transitions in high-pressure ϵ-FeOOH are studied using density functional theory calculations including an on-site Coulomb repulsion term. A high-spin to low-spin transition in trivalent iron is predicted at $\sim$ 58 GPa, in agreement with previous theoretical study [1] and experimental indications [2]. The spin transition is heralded by a second order $P2_1$nm to Pnnm phase transition at $\sim$ 43 GPa, driven by hydrogen bond symmetrization at the critical hydrogen bond $O \cdots O$ limit of $\simeq$ 2.4 Å. Our results give indications of a possible connection between the symmetry of hydrogen bonds in ϵ-FeOOH and the spin state of Fe^{3+}, with important implications in disclosing the influence of water content in the mantle redox state.

Funding by DFG SPP1236 (PE883/8-1) is acknowledged.

[1] Otte et al. Phys. Rev. B **80**, 205116 (2009).
[2] Gleason et al. In preparation.

O 51.13 Wed 19:15 H36

From spheres to iso: Implementing implicit solvation in FHI-aims — •Ran Jia, Chunsheng Liu, Daniel Berger, Harald Oberhofer, and Karsten Reuter — Department Chemie, Technische Universität München, Lichtenbergstr. 4, D-85747 Garching, Germany

At the cost of reduced accuracy, implicit solvation models yield strong speedups compared to explicit solvent simulations. Here, we report on the implementation of the multipole moment expansion (MPE) solvent continuum model into the density-functional theory (DFT) program package FHI-aims. Characterizing the surrounding solvent mainly by its dielectric constant and density, the form of the cavity employed for the solute and the description of the reaction field created by the polarized solvent are the two central characteristics of any implicit solvation approach. In MPE the reaction field is computed as a truncated multipolar expansion. In our implementation we discard the prevalent cavity representation in form of a set of overlapping spheres centered around the solute atoms in favor of an electron isodensity surface. This allows for more flexible shapes with increased physical meaning. In particular, it paves the way towards the description of one- or two-dimensional periodic systems, and therewith to complex solid-liquid interfaces.

O 52: Organic/bio Molecules on Metal Surfaces V

Time: Wednesday 16:00–19:00 Location: H38

O 52.1 Wed 16:00 H38

Steering on-surface self-assembly of high-quality hydrocarbon networks with terminal alkynes — •Nenad Kepčija[1], Yi-Qi Zhang[1], Martin Kleinschrodt[1], Jonas Björk[2], Svetlana Klyatskaya[3], Florian Klappenberger[1], Mario Ruben[3,4], and Johannes V. Barth[1] — [1]Physik Department E20, Technische Universität München, James-Franck-Straße, 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 — [4]IPCMS-CNRS, Universite de Strasbourg, 23 Rue de Loess, 67034 Strasbourg, France

The 2D self-assembly of 1,3,5-triethynyl-benzene (TEB) and *de novo* synthesized 1,3,5-tris-(4-ethynylphenyl)benzene (Ext-TEB) on Ag(111) was studied by means of scanning tunneling microscopy (STM) under ultra-high vacuum (UHV) conditions. Both molecules form nanoporous networks exhibiting organizational chirality, mediated by novel, planar six-fold cyclic binding motifs. Comparison with bulk structures of similar molecules suggests that these motifs appear only in 2D environments. The key interaction is identified as $C–H \cdots \pi$ bonding. For Ext-TEB an additional open-porous phase exists. The nature of the underlying non-covalent bonding schemes is analyzed by the density functional theory (DFT) calculations. Comparison of the calculations focusing on isolated 2D molecular sheets and those including the substrate reveals the delicate balance between molecule-molecule and molecule-substrate interactions.

O 52.2 Wed 16:15 H38

Differences in Chiral Expression: Racemic and Enantiopure Heptahelicenes on Various Metal Surfaces — •Johannes Seibel[1] and Karl-Heinz Ernst[1,2] — [1]Empa, Nanoscale Materials Science, Dübendorf, Switzerland, Dübendorf, Switzerland — [2]University of Zürich, Zürich, Switzerland

Previous scanning tunneling microscopy (STM) studies[1,2,3] of racemic and enantiopure heptahelicenes (rac-[7H], M-[7H] or P-[7H]) on Cu(111) showed the formation of mirror domains. However, these domains consist of both enantiomers in an equal ratio and naturally, pure M- and P-[7H] form different structures. To investigate the influence of the metal surface on the two-dimensional ordering of heptahelicenes, we deposited rac-[7H] and M-[7H] on Cu(100), Ag(111) and Au(111). STM measurements reveal different expressions of chirality. On Ag(111) and Au(111) rac-[7H] forms a double-row structure similar to Cu(111), but no enantiomorphous domains are observed. Additionally, the structures of M-[7H] are very similar to the ones observed on Cu(111). In contrast to the structures on the 111-terminated surfaces containing both heptahelicene enantiomers, rac-[7H] on Cu(100) separates into enantiomorphous domains containing only M-[7H] or P-[7H], respectively.

[1] R. Fasel, M. Parschau and K.-H. Ernst, Nature 2006, 439, 449-452 [2] R. Fasel, M. Parschau and K.-H. Ernst, Angew. Chem. Int. Ed. 2003, 42, 5178-5181 [3] M. Parschau, R. Fasel and K.-H. Ernst, Cryst. Growth & Des. 2008, 8, 1890-1896

O 52.3 Wed 16:30 H38

Stereochemistry of C_4 dicarboxylic acids on Cu(110) — •Chrysanthi Karageorgaki[1] and Karl-Heinz Ernst[1,2] — [1]EMPA, Nanoscale Materials Science, Dübendorf, Switzerland — [2]Chemistry department, University of Zürich, Zürich, Switzerland

In order to better understand self assembly at the molecular level, we are studying different chiral butanedioic acids, like tartaric acid (TA), malic acid (MA) and 2,3-dimethyl succinic acid (DMSU), as well as achiral analogues like succinic acid (SU), maleic acid (MEA), fumaric acid (FUA), meso-DMSU and trans 1,2-cyclohexane dicarboxylic acid (CHDCA) on Cu(110). Here we present LEED, STM and TPD results of the aforementioned compounds. Apart from coverage dependent "surface explosion" decomposition, all achiral compounds undergo chiral symmetry breaking, observed as superposition of mirror domains in LEED. Interestingly, the obtained LEED structures coincide for the various compounds, suggesting that the chiral recognition at surfaces derives from the substrate, in particular, when the molecule doesn't have functional groups to form strong intermolecular bonds. STM reveals that the substrate is "etched", leading to chiral reconstructions of the surface.

O 52.4 Wed 16:45 H38

Orientation- and site-dependent electronic structure of a molecule on Au(111) investigated by STM and DFT with dispersion corrections — •Maya Lukas[1], Karin Fink[1], Kerrin Dössel[1], Alexandrina Schramm[1], Christophe Stroh[1], Olaf Fuhr[1], Marcel Mayor[1,2], and Hilbert von Löhneysen[1,3] — [1]Karlsruher Institut für Technologie (KIT), Institut für Nanotechnologie, D-76021 Karlsruhe — [2]Universität Basel, Department of Chemistry, CH-4056 Basel — [3]Karlsruher Institut für Technologie (KIT), Physikalisches Institut und Institut für Festkörperphysik, D-76021 Karlsruhe

The exact orientation and bonding of a molecular wire to the connecting electrodes has a crucial effect on the conductance. Determining the exact bonding configuration as well as the electronic properties in the same experiment is hardly ever achieved, if possible at all.

We investigated a molecule that consists of three identical molecular wires connected in a rigid conformation. Due to the molecules chiral form the wires become different when coupled to a Au(111) surface. By scanning tunneling microscopy and density functional theory with dispersion corrections we study the local electronic structure of the molecular wires. We find strong variations of the electronic structure for wires with different orientation with respect to the surface within one molecule. Furthermore, the effect a positional shift of the whole molecule on the surface is investigated. From our calculations we are able to distinguish effects due to structural rearrangements in the molecule from effects due to electronic interaction with the surface.

O 52.5 Wed 17:00 H38

From achiral molecules to chiral superstructures: triphenylamine derivatives on Au(111) — •Kathrin Müller[1], Stefano Gottardi[1], Juan Carlos Moreno-Lopéz[2], Klaus Müllen[3], Milan Kivala[4], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Centro Atómico Bariloche-Instituto, Balseiro-CNEA-UNCuyo-CONICET, Río Negro, Argentina — [3]Max Planck Institute for Polymer Research, Mainz, Germany — [4]Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Germany

We investigated the self-assembly of achiral triphenylamine derivatives, so-called heterotriangulenes, which feature cyano functionalities intended for intermolecular dipolar coupling, on Au(111). We observed the coexistence of two phases, both expressing chirality. Deposition of one monolayer leads to the formation of a hexagonally closed packed phase. For submonolayer coverage numerous vacancies are present, which organize spontaneously forming a porous network. The second phase is stabilized by the introduction of metal-coordinated bonds and also exhibit pores. The structural models of the different binding motives of these two phases, the intermolecular interactions as well as the influence of the substrate on the assembly will be discussed. Moreover, we investigated the effect of post-annealing onto the assembly structure. We observed a partial transformation of one phase into the other. This spontaneous assembly of molecules into chiral and porous network structures on surfaces is of great interest for many future applications for example in catalysis, opto-electronics or as sensors.

O 52.6 Wed 17:15 H38

On-surface polymerization of biphenyl derivatives on Ag(111) — •Fei Song[1], Tuan Anh Pham[1], Serpil Boz[2], Umut Soydaner[3], Marcel Mayor[3], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, 9747AG, the Netherlands — [2]Department of Physics, University of Basel, Switzerland — [3]Department of Chemistry, University of Basel, Switzerland

The controlled assembly of molecular building blocks, which possess functional units for switching, subsequent covalent interlinking etc., into functional architectures on surfaces has become an established research fields over the past decades [1]. However, the structures which are based on non-covalent interactions mostly lack mechanical stability. In view of possible future applications higher stability and the prospect of improved charge transport are important requirements. In this work, a unique concept to control both the molecular self-assembly and the subsequent intermolecular coupling was utilized through equipping the molecular building blocks with terminal protecting groups. Specifically, biphenyl derivatives with BOC protecting groups were deposited onto a Ag(111) surface. STM and XPS were used to explore both the self-assembly behaviors and the on-surface polymerization after annealing the sample at elevated temperatures. It turned out that the protecting groups can be split off by annealing [2] and the deprotected monomers interlink into polymeric structures. By tuning the design of the organic monomers, the reactivity as well as the size of polymeric structures can be controlled. Reference [1] J.A.A.W. Elemans, Angew. Chem. Int. Ed. 48 (2009) 7298 [2] S. Boz et al., Angew. Chem. Int. Ed. 48 (2009) 3179

O 52.7 Wed 17:30 H38

Self-assembly of a threefold symmetric CN-terminated molecular linker on Cu(111) and Ag(111) — •Peter B. Weber[1], Yiqi Zhang[1], Florian Klappenberger[1], Svetlana Klyatskaya[2], Mario Ruben[2,3], and Johannes Barth[1] — [1]Physik Department E20, Technische Universität München, Garching 85748, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology — [3]Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg

We present a scanning tunneling microscopy study of the self-assembly of 1,3,5-tri(4-cyanophenyl)-benzene (TCB) on the Cu(111)-surface and on the Ag(111)-surface. The measurements were carried out under ultra-high-vacuum conditions at 5.5 K. On both surfaces the formation of large regular networks was observed. The molecules are arranged in a hexagonal lattice and the islands are stabilized by multiple proton acceptor ring interactions [1]. This behavior contrasts that for linear NC-Ph$_x$-CN species where multiple nanoporous networks were formed partially involving dipolar interactions [2]. The formed networks are commensurable with the Cu(111)-surface but not with the Ag(111)-surface. In a second step we demonstrate the usefulness of these islands to steer the positioning of Co-atoms resulting in a high yield of Co-phenyl half-sandwich compounds with potentially interesting magnetic properties.

[1] Arras, E. et al, Phys. Chem. Chem. Phys. 14, 15995 (2012) [2] Kühne, D. et al, J. Phys. Chem. C 113, 17851 (2009)

O 52.8 Wed 17:45 H38

The metal | ionic liquid interface: Adsorption behavior of ionic liquid adlayers on Cu(111) — Stephan Gabler[1,2], •Benedikt Uhl[1,2], Florian Buchner[1,2], and R. Jürgen Behm[1] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — [2]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89069 Ulm, Germany

Ionic liquids (IL's) are promising electrolytes in Li-Ion batteries. The behavior of IL's at the electrode | electrolyte interface is crucial for the performance of such electrochemical systems, studies on this topic, however, are at their very beginning. In this work, we investigated the adsorption behavior of 1-Butyl-1-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide (BMP TFSA) on Cu(111) in the submonolayer and monolayer range. Combined STM and XPS investigations were conducted under UHV conditions and at temperatures between 100 K and 298 K. Compared to the XPS bulk signals, additional peaks are found in the N1s and S2p region for thin BMP-TFSA adlayers. The additional S2p peak indicates a sulfidic species on the surface (e.g. Cu2S), which we assume is due to a partial decomposition of the anion. In STM, two different structures are observed on the surface: the first is stable at room temperature and the second is solely found below 170 K. Additionally the Cu-steps are altered, which indicates the participation of the metal surface in the decomposition reaction. Presumably, the first structure represents decomposition products and the second one intact IL molecules.

O 52.9 Wed 18:00 H38

The metal | ionic liquid interface: Comparison of the adsorption behavior of different ionic liquids on Ag(111) — •Florian Buchner[1,2], Benedikt Uhl[1,2], Dorothea Alwast[1,2], Hsinhui Huang[1,2], and Rolf-Jürgen Behm[1,2] — [1]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89069 Ulm, Germany — [2]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Ionic liquids are promising candidates as electrolytes in Li-ion batteries, which play a key role in energy storage devices. In this model approach, we aim towards a molecular understanding of the processes at the metal electrode | ionic liquid interface. 1-butyl-1-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide $[BMP]^+[TFSA]^-$ and 1-ethyl-3-methylimidazolium-bis(trifluoromethylsulfonyl)imide $[EMIM]^+[TFSA]^-$ on Ag(111) are studied at mono- and submonolayer coverages by scanning tunneling microscopy (STM) under UHV conditions in the temperature range between 100 K and room temperature. $[BMP]^+[TFSA]^-$ exists in a highly mobile 2D gas phase in the range between 300 K and 100 K, i.e., it exhibits a low diffusion barrier. Additionally, at 100 K a long-range ordered and homogeneous 2D solid phase fills up large terraces, and a 2D disordered phase is found close to steps. Dynamic STM measurements highlight exchange of adspecies at the phase boundary between 2D solid and 2D gas phase. The adsorption behavior of $[BMP]^+[TFSA]^-$ and $[EMIM]^+[TFSA]^-$ on Ag(111) is discussed, focusing on ordering aspects, diffusion properties and 2D melting.

O 52.10 Wed 18:15 H38

An explicit solvation model for the force field description of bis(terpyridine) adsorption — •Daniela Künzel and Axel Gross — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

In the theoretical modeling of organic adlayers that are deposited from solution the solvent is typically not taken into account.[1] Instead, calculations are often carried out at the solid/vacuum interface. DFT and force field simulations of bis(terpyridine) (BTP) adsorption have shown that even such a simple model is able to reproduce and explain experimental observations made at the solid/liquid interface.[2] However, any effects the solvent might have on the system remain unknown.

Thus we now present the use of an explicit solvation model for the force field simulation of the ordered BTP adsorption on graphite. Even though different force fields yield different quantitative values for the energetics of the molecules in solution, the effect of solvation can at least be distinguished in a qualitative way.

The calculations show that solvation has a significant effect on the thermochemistry of BTP adsorption. Properties of the ordered adsorbate layers are also affected by these changes. Finally, taking solvation into account can also help to gain a deeper understanding of the structure formation process.

[1] Kucera, J.; Groß, A. *Langmuir* **2008**, *24*, 13985.

[2] Meier et al. *J. Phys. Chem. C* **2010**, *114*, 1268-1277. Künzel et al. *Phys. Chem. Chem. Phys.* *2009*, *11*, 8867-8878.

O 52.11 Wed 18:30 H38

The role of dispersion forces in SAM(aromatic thiolates)/Au(111) systems: a DFT study including semiempirical dispersion corrections — •Jan Kučera and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm, Germany

The anchoring of aromatic thiolates on metal substrates has been widely used as a feasible method to effectively modify the electronic properties of environment/metal interfaces intended as, e.g., components of new nanoelectronic devices. The theoretical description of those systems represents a rather complex task since also noncovalent effects as, e.g., van der Waals (vdW) interactions operate in the formation of the complexes.

We performed periodic density functional theory (DFT) calculations with semiempirical DFT-D3 [1] and DFT+vdW [2] corrections to clarify the role of dispersion in the molecule-surface as well as in the molecule-molecule interaction. To be specific, we addressed SAM/Au(111) complexes with the SAM formed by di-4-pyridine-di-sulphide (PySSPy), 4-mercaptopyridine (SPy), and 4-(4-mercaptophenyl) pyridine (SPhPy) molecules. We find that the stability of the PySSPy/Au complex is dominated by dispersion. In contrast, covalent bonding is the structure- and stability-determining factor in SPy and SPhPy/Au complexes, where dispersion only significantly contributes to the molecule-substrate interaction.

[1] S. Grimme et al., J. Chem. Phys. **132**, 154104 (2010).

[2] A. Tkatchenko and M. Scheffler, PRL **102**, 073005 (2009).

O 52.12 Wed 18:45 H38

DFT Studies on the Adsorption of Atomic Sulfur and Methanethiolate at the Cu(111) Surface — •Porntip Seema, Jörg Behler, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum

Density-functional theory (DFT) calculations have been employed to study the adsorption of atomic sulfur and methanethiolate at the Cu(111) surface. A large number of surface models has been investigated considering a variety of adsorbate phases, binding sites and surface coverages. The results show that the adsorption of atomic sulfur and methanethiolate gives rise to surface reconstructions. The most preferable phase for atomic sulfur contains three sulfur atoms in the unit cell and three copper atoms in the reconstructed layer. For methanethiolate, several similar local minima exist differing in the positions of copper atoms in the reconstructed layer and these calculated structures deviate from the perfect fourfold Cu-S coordination observed in STM. Furthermore, modifying the chemical composition of the relaxed layer, e.g. by adding another copper atom, yields structures of comparable stability.

O 53: Scanning Probe Methods II

Time: Wednesday 16:00–19:15 Location: H31

O 53.1 Wed 16:00 H31

Driving a Macroscopic Oscillator with the Stochastic Motion of a Hydrogen Molecule — •Christian Lotze[1], M. Corso[2], K.J. Franke[1], F. v. Oppen[1,3], and J.I. Pascual[2,4] — [1]Freie Universität Berlin — [2]CIC nanoGUNE, Donostia-San Sebastián, Spain — [3]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin — [4]IKERBASQUE, Bilbao, Spain

Tuning Fork based STM/AFM is a well-established method combining the advantages of scanning tunneling and dynamic force microscopy, allowing stable imaging with tip oscillation amplitudes below 1 Å. In this way, conductance and Δf measurements of molecular junctions can be obtained simultaneously [1] with intramolecular resolution [2].

One of the most intriguing aspects of molecular junctions relates to the effect of structural bi-stabilities in the properties of the junction. These lead, for example, to conductance fluctuations, telegraph noise and the possibility of switching the electrical transport through the junction. In this presentation, we characterize H_2 molecules on Cu(111), a model bi-stable molecular system, using dynamic force spectroscopy. The effect of current-induced stochastic fluctuations of conductance is correlated with fluctuations in force. In our experiment, we identified the latter from frequency shift and energy dissipation measurements, picturing a regime in which electrical transport and mechanical motion are coupled in a concerted dynamics that drives the system into self-oscillation [3].

[1] Fournier, *et al*, PRB 84, 035435 (2011) [2] Gross *et al*, Science 324, 1428 (2009) [3] C. Lotze *et al*, Science 338, 779 (2012)

O 53.2 Wed 16:15 H31

Improvement of STM Resolution with H-sensitized Tips — Jose Ignacio Martínez[1], •Enrique Abad[1,2], César González[1], Fernando Flores[1], and José Ortega[1] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain — [2]Computational Biochemistry Group, Institut für Theoretische Chemie, Universität Stuttgart, Stuttgart, Germany

The improvement of spatial resolution in STM is attaining a lot of attention in diverse fields such as Surface Science [1]. In particular, recent Scanning Tunneling Hydrogen Microscopy (STHM) experiments on PTCDA/Au(111) have shown unprecedented intramolecular and intermolecular spatial resolution [1]. In our work, we analyze the effect on the STM images of hydrogen interacting with tip or sample, using an accurate STHM theoretical simulation technique [2]. Notice that the standard Tersoff-Hamman approach cannot take into account the influence of the hydrogen in the STM image.

We find that the STHM resolution enhancement is due to atomic H adsorbed on the tip [3]. The adsorbed H-atoms induce important changes in the Density of States (DOS) at the Fermi level (E_F) of the tip, increasing its total value, and making it more directional. Also, due to the interaction with the tip, E_F is shifted to the middle of the PTCDA LUMO peak, increasing the DOS of the sample at E_F [3].

[1] L. Gross, Nat. Chem. 3, 273 (2011).

[2] J. I. Martínez, E. Abad, et al. Org. Electron. 13, 399 (2012).

[3] J. I. Martínez, E. Abad, et al., Phys. Rev. Lett. 108, 246102 (2012).

O 53.3 Wed 16:30 H31

Mapping the surface adsorption potential with the scanning tunneling microscope — •Georgy Kichin[1,2], Christian Wagner[1,2], Stefan Tautz[1,2], and Ruslan Temirov[1,2] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Germany

We propose a new method that allows us to study the adsorption behavior of molecular hydrogen or deuterium on the surface with atomic scale resolution. First, the molecular gas is condensed in the junction of the low-temperature scanning tunneling microscope (LT STM). Passing the tunneling current through the junction the vibrational excitations of the molecules are induced by inelastically scattered electrons. By mapping the inelastic excitation energy along the surface we obtain the information that is related to the local adsorption potential of the gas molecules on this surface. We will discuss how this information can be used to reconstruct the quantitative information about the surface adsorption potential.

O 53.4 Wed 16:45 H31

Voltage pulse shapes in time-resolved STM measured with photons — •Markus Etzkorn[1], Christoph Grosse[1], Klaus Kuhnke[1], Sebastian Loth[1,2], and Klaus Kern[1,3] — [1]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Center for Free-Electron Laser Science, 22761 Hamburg, Germany — [3]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Time-resolved STM measurements using electronic pulses enable the study of local dynamics in the ns-regime and below [1]. One necessary prerequisite for such measurements is the knowledge of the time-dependance of the transient bias voltage V(t) at the tunnel junction. Due to the high frequency limitations of the wiring and the impedance mismatches in the experiments, perfect pulses fed into the STM will deviate from perfectness when they reach the tunnel junction. Here we introduce a new concept that enables the direct measurement of the true transient bias voltage in the junction using the characteristic photon signal created by plasmon decay between tip and sample. It relies on the fact that both plasmon decay and photon detection are fast on the time scale of the variation of V(t). We proof that this method gives correct results by redundant measurements of the autocorrelation using an all-electronic pump-probe scheme. Over and above we show how this method can be used to characterize the transfer function of a given set-up, and how one can optimize the transient bias shape by chirp modulation of the applied pulses. [1] S. Loth, M. Etzkorn, C.P. Lutz, D.M. Eigler, A.J. Heinrich, Science **329**, 1628 (2010).

O 53.5 Wed 17:00 H31

Investigation of the stiffness of the BN-nanomesh by combined STM and AFM measurements at low temperatures

— •Tobias Herden[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 des Nanostructures, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The single layer boron-nitride nanomesh on Rh(111) [1] was intensively investigated by an homebuilt combined STM-AFM operating in the qPlus setup [2] at low temperatures with sub-nm oscillation amplitudes. From 3D-frequency shift data we calculated the energy landscape and lateral and vertical forces acting between the tip and the BN-layer. Slight variations in the forces between the (top, hcp)- and the (fcc, hcp)-sites (i.e. the different alignments of the rim sites of the hexagonal corrugation in respect to the Rh surface) enable us to derive stiffness properties of the highly corrugated layer. Our local results are further supported by statistical evaluation of atomic-scale AFM measurements of the lateral displacement of the BN-hexagons. To get a more profound understanding of the mechanical properties of the insulating single layer system, our experimental findings are compared with theoretical calculations by Laskowski et al. [3,4].

[1] M. Corso, Science 202, 217 (2004)
[2] F. J. Giessibl, Appl. Phys. Lett. 73, 3956 (1998)
[3] R. Laskowski et al., Phys. Rev. Lett. 98, 106802 (2007)
[4] R. Laskowski et al., Phys. Rev. B 81, 075418 (2010)

O 53.6 Wed 17:15 H31

Nanoscale imaging of photoelectrons using an atomic force microscope

— •Ping Yu[1] and Jürgen Kirschner[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Von-Danckelmann-Platz 3, D-06120 Halle, Germany

Photoemission current imaging at the nanoscale is demonstrated by combining an atomic force microscope (AFM) with laser excitation of the tip-sample gap. Photoelectrons emitted from the sample are collected by the AFM tip while the tip-sample distance is precisely controlled by the van der Waals force between them. We observe pronounced photoemission current contrast with spatial resolution of 5 nm on a cesium covered Au(111) surface, which is better than its corresponding AFM topography resolution. This high spatial resolution of the photoemission current image can be attributed to the strong dependence of the local potential barrier on the tip-sample distance. Our experiments provide a method for photoelectron imaging with high spatial resolution and extend the functionality of state-of-the-art scanning probe techniques.

O 53.7 Wed 17:30 H31

The effect of sample resistivity on Kelvin probe force microscopy

— •Alfred J. Weymouth and Franz J. Giessibl — University of Regensburg, 93040 Regensburg, Germany

Kelvin probe force microscopy (KPFM) is a powerful technique to probe the local electronic structure of materials with atomic force microscopy. One assumption often made is that the applied bias drops fully in the tip-sample junction. We have recently identified an effect, the Phantom force, which can be explained by an ohmic voltage drop near the tip-sample junction causing a reduction of the electrostatic attraction when a tunneling current is present. Here, we demonstrate the strong effect of the Phantom force upon KPFM that can even produce Kelvin parabolae of opposite curvature.

Appl. Phys. Lett., 101, 213105 (2012)

O 53.8 Wed 17:45 H31

Three dimensional scanning lifetime microscopy using diamond

— •Philip Engel, Andreas W. Schell, and Oliver Benson — Humboldt-Universität zu Berlin, AG Nanooptik

Knowledge of the local density of optical states (LDOS) is important for the design of nanoscale enviroments for controlled light matter interaction. Here, we use the nitrogen vacancy (NV) defect center in nanodiamond as nanoscale probe for the LDOS. The NV defect center has a long-term stability even at room-temperature, which makes it an ideal candidate as a pointlike probe glued on an atomic force microscopy tip. Due to Fermi's golden rule the LDOS can be directly measured via lifetime changes of an emitter. Recently this was shown with fluorescent dye beads in two dimensions [1]. Our technique allows for the measurement of the LDOS in all three dimensions and the single emitter character of our probe avoids inhomogeneous broadening from ensemble averaging.

[1] M. Frimmer et al., Phys.Rev.Lett. 107, 123602 (2011).

O 53.9 Wed 18:00 H31

Utilizing dynamic work function measurements to distinguish adsorbates on Si(100)

— •Ferdinand Huber, Alfred J. Weymouth, and Franz. J. Giessibl — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

It has been proposed that STM with an oscillating tip can be used to measure the work function locally [1, 2]. By combining this technique with STM and AFM measurements, taken in UHV at room temperature, we should be able to distinguish between deposited adatoms and surface defects [3]. Here, we deposit Mo on Si(100) and attempt to determine its atomic structure and true adsorption sites at low coverage as there are open questions [4].

[1] J. B. Pethica, J. Knall and J. H. Wilson, Inst. Phys. Conf. Ser. **134**, 597 (1993)
[2] M. Herz, Ch. Schiller, F. Giessibl and J. Mannhart, Appl. Phys. Lett. **86**, 153101 (2005)
[3] R. J. Hamers and U. K. Köhler, J. Vac. Sci. Technol. A **7**, 2854 (1989)
[4] P. Bedrossian, Surface Science **320**, 247 (1994)

O 53.10 Wed 18:15 H31

Probing the probe: tip front atom characterization

— •Florian Pielmeier and Franz J. Giessibl — Institut für experimentelle und angewandte Physik, Universität Regensburg

The angular dependence of the chemical bonding forces between a tungsten (W) tip and a carbon monoxide molecule adsorbed on Cu(111) has been demonstrated recently by means of atomic force microscopy [1]. Single , dual or tiple minima in the force profile for W tips have been observed. They originate from the different charge density distributions at the apex of the tungsten tip, resembling the high symmetry directions of the bcc crystal lattice [2]. Furthermore absolute values for the interaction forces can be given by 3D force spectroscopy [3]. Here we present data for different tip materials (iron, copper and tungsten), analyzing the different symmetries and forces allows then the identification of the foremost tip atom. This enables a detailed interpretation of experimental data. As the characterization experiment itself is rather straightforward, this method, called carbon monoxide front atom identification (COFI), can be used in general to characterize the probe prior and/or after any experiment.

[1] J. Welker, F.J. Giessibl, Science, 336, 444 (2012) [2] C. A. Wright, S. D. Solares, Nanoletters, 11, 5026 (2011) [3] H. Hölscher, S.M. Langkat, A. Schwarz, R. Wiesendanger, Applied Physics Letters, 81, 4428 (2002)

O 53.11 Wed 18:30 H31

Theoretical Scanning Probe Images of the (001) Surfaces of MnO and NiO

— •Mihail Granovskij[1,2], Andreas Schrön[1,2], and Friedhelm Bechstedt[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]ETSF

In the paramagnetic state the ground-state crystal structure of the

3d transition metal oxides (TMOs) MnO and NiO is given by an ideal rock-salt (rs) structure. Below their respective Néel temperature, however, it is characterized by the formation of an antiferromagentic ordering AFM2 which is acompanied by a rhombohedral distortion along the [111] direction. The intersection of the thermally swichable magnetic ordering AFM2 with the crystal surfaces makes TMO surfaces ideal benchmark materials for the investigation of recent magnetic scanning probe techinques such as spin-polarized scanning tunneling microscopy (SP-STM) and magnetic exchange force microscopy (MExFM).

We present a density functional theory (DFT) study of the (001) surfaces of MnO and NiO inculding an on-site interaction U. Different theoretical approaches for the description of magnetic scanning probe techniques are employed. the magnetic tip is modelled by a single Fe or 5-Fe-atom pyramid. For NiO, the calculated scanning probe images explain the spin contrast and the corrugation found experimentally. For MnO, the calculated images represent interesting predictions which differ from that of NiO.

O 53.12 Wed 18:45 H31

Scanning Microwave Microscopy combined with Amplitude Modulation Atomic Force Microscopy — •Matthias A. Fenner — Agilent Technologies, Lyoner Str. 20, 60528 Frankfurt

We report the implementation of a Scanning Microwave Microscopy (SMM) in Amplitude Modulation Atomic Force Microscopy (AFM) [1]. SMM combines AFM and a Vector Network Analyzer using microwave tip sample interactions to characterize dielectric and electronic material properties on the nanometer scale. The method employs contact mode AFM to yield calibrated capacitance and dopant density values and is described in detail by Huber et al. [2].

The extension of the method to Amplitude Modulation AFM offers several benefits:

1. It can be applied to very soft matter or nanosize objects which are poorly bound to a substrate surface.
2. It can be combined with advanced AC mode techniques like Kelvin Force Microscopy for surface potential measurements or Magnetic Force Microscopy.

We report a feasibility study for this novel technique.

[1] Amplitude Modulation Atomic Force Microscopy, R. Garcia, Wiley-VCH (2010)

[2] H. P. Huber et. al, Rev. Sci. Instrum. 81, 113701 (2010)

O 53.13 Wed 19:00 H31

Infrared nanoscopy of biomaterials — Adrian Cernescu[1,2], Sergiu Amarie[2], Tobias Geith[3], Stefan Milz[4], and •Fritz Keilmann[1] — [1]Ludwig-Maximilians-University and Center for NanoScience, Garching, Germany — [2]Neaspec GmbH, Martinsried, Germany — [3]Ludwig-Maximilians-University, Institute for Clinical Radiology, Munich, Germany — [4]Ludwig-Maximilians-University, Department of Anatomy, Munich, Germany

Spectroscopic near-field imaging is enabled by combining 20nm-resolving tip-scattering near-field microscopy (s-SNOM) with an infrared continuum source. Specific contrasting of biomineral components is enabled by simply choosing the appropriate "fingerprint" infrared region that as in traditional FTIR (Fourier-transform infrared spectroscopy) identifies virtually any chemical compound. Hence nano-FTIR stands for the successful realization of combining s-SNOM and FTIR [1].

The investigated samples are nanocomposite biomaterials, namely human bone sections, human tooth specimens and mollusk shell which contain mineral nanocrystals in organic matrices [2]. The mineral parts are highlighted by their resonantly enhanced contrast due to phonons.

Our method is surface-sensitive, probing to a depth of about 30 nm. It should be straightforwardly applicable in many fields of general mineralogy, solid state research, and materials science.

[1] S. Amarie, T. Ganz, and F. Keilmann, Opt. Express 17, 21794 (2009); [2] S. Amarie, P. Zaslansky, Y. Kajihira, E. Griesshaber, W.W. Schmahl and F. Keilmann, Beilstein J. Nanotechnol. 3, 312 (2012).

O 54: Organic Electronics and Photovoltaics (jointly with CPP, DS, HL)

Time: Wednesday 16:00–19:00 Location: H33

O 54.1 Wed 16:00 H33

Effects of nuclear dynamics on light absorption, charge injection, recombination, and dye regeneration conditions in dye-sensitized solar cells — •Sergei Manzhos[1], Hiroshi Segawa[2], and Koichi Yamashita[3] — [1]Department of Mechanical Engineering, National University of Singapore, Blk EA #07-08, Singapore 117576 — [2]RCAST, University of Tokyo, 4-6-1, Komaba, Meguro-ku, Tokyo 153-8904, Japan — [3]Department of Chemical System Engineering, University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

We present molecular dynamics studies of effects of nuclear motions on light absorption and charge injection, recombination, and dye regeneration conditions for two organic dyes adsorbed on anatase (101) surface of TiO2 in mono- and bi-dentate configurations. We studied the effects of temperature, deuteration, and co-adsorbed water. Averaged over nuclear motions driving forces for injection and regeneration can differ significantly from their static estimates computed in most works. As a result, injection rate could be different by orders of magnitude. As the expectation value of the ground state energy is higher than its optimum geometry value (by up to 0.1 eV), nuclear motions will affect dye regeneration by recently proposed redox shuttle-dye combinations operating at low driving forces. Dye orientation motions are predicted to increase back-donation rate by orders of magnitude. Dye structure, adsorption mode, and the presence of water affect strongly the dynamics of energy level matching. Temperature in the range of 300-350K and deuteration have little effect on driving forces but red-shift of the absorption spectrum by a few %.

O 54.2 Wed 16:15 H33

Photoemission Studies of Highly Reactive Organic Photosensitizers — •Mathias Fingerle[1], Maximilian Hemgesberg[2], Yvonne Schmitt[2], Sebastian Schmitt[2], Dimitri Imanbaew[2], Harald Kelm[2], Eugen Risto[2], Stefan Lach[1], Markus Gerhards[2], Christoph van Wüllen[2], Werner Thiel[2], and Christiane Ziegler[1] — [1]Fachbereich Physik, Erwin-Schrödinger-Str. 56, D-67663 Kaiserslautern, Germany — [2]Fachbereich Chemie, Erwin-Schrödinger-Str. 52, D-67663 Kaiserslautern, Germany

Substituted phenothiazines (PTs) are promising candidates for applications in the field of organic electronics. Due to the fact, that the electronic, magnetic and geometrical properties of the phenothiazine compared to its radical cation differ substantially, PT redox couples are of great interest for organic devices like dye sensitized solar cells (DSSCs). Here, the electronic properties of N-substituted phenothiazine dyes derived from 3.8-dithien-2-ylphenothiazine (DTPT), among them the first PT containing an olefinic moiety with an electron withdrawing group close to the nitrogen atom, were probed via photoemission spectroscopy. The thin film growth of the dyes and their oxidized species after spin coating was analyzed by X-ray photoelectron spectroscopy (XPS) and qualitatively visualized by scanning force microscopy (SFM). Through UV-photoelectron spectroscopy (UPS) and inverse photoelectron spectroscopy (IPES), the occupied and unoccupied energy levels could be attained and compared to data acquired by UV/Vis spectroscopy and DFT calculations. It is shown, that chemical oxidation by NOBF4 leads to a dramatic decrease of the band gap.

O 54.3 Wed 16:30 H33

Investigation of the electronic structure of phosphorescent Platinum(II) complexes on Au(111) by STM and STS — •Pascal Raphael Ewen, Hasmik Harutyunyan, Jan Sanning, Matteo Mauro, Cristian Alejandro Strassert, and Daniel Wegner — Physikalisches Institut - Westfälische Wilhelms Universität Münster

Quenching effects still limit the efficiency of state-of-the-art organic light emitting diodes (OLEDs) at higher doping concentrations of the triplet emitter molecules within the emission layer. A possible candidate for avoiding of the loss of luminescence are recently synthesized Pt(II) complexes that do not show quenching even when aggregated into fibers or gels. The efficient implementation of such complexes in electronic devices requires a fundamental understanding of the interaction of the molecules with the local environment. A systematic investigation of the adsorption and the electronic structure of slightly different phosphorescent Pt(II) complexes offers information about the influence of ligands and substituents on the complexes as well as their interactions with neighbours and the substrate. We have studied the impact of molecule-surface and intermolecular interactions on the self-assembly and electronic structure of Pt-complex monolayers on Au(111) using scanning tunneling microscopy (STM) and spectroscopy (STS) at low temperature. By determining energies and spatial distributions of several frontier orbitals, we are able to evaluate the impact of hybridization on the molecular electronic structure with important consequences for the optical properties.

O 54.4 Wed 16:45 H33

Overcoming the limitations of work-function modifications induced by adsorption of self-assembled monolayers — •Oliver T. Hofmann, Yong Xu, Patrick Rinke, and Matthias Scheffler — Fritz-Haber Institut der MPG, Berlin, Germany

Controlling the work function of electrodes critically determines charge-injection barriers and is of high importance for organic electronic devices. Such control can be easily achieved by adsorbing dipolar self-assembled monolayers. Despite the common application of this method, its limitations remain largely unexplored. It has, however, been demonstrated that charge-transfer occurs as soon as the molecular LUMO comes into resonance with the Fermi-energy when the molecular dipole moment is systematically increased by adding multiple repeat units. This Fermi-level pinning limits the achievable work-function modification. In turn, we argue that molecules with negative electron affinities never reach this limit and can reduce the work-function in principle all the way down to zero. As a proof of concept, we study the interaction between the ZnO$(10\bar{1}0)$ surface and pyridine using hybrid density functional theory with a variable fraction of exact exchange and a correction scheme for screened van-der-Waals forces. In agreement with experimental observations, we find an adsorption-induced work-function reduction of up to -2.9 eV. For a hypothetical ultra-dense pyridine monolayer the work-function reduction could even reach -4.3 eV for this surface.

O 54.5 Wed 17:00 H33

Surface electronic structure and electron dynamics for pristine and adsorbate-covered ZnO$(10\bar{1}0)$ — •Jan-Christoph Deinert, Daniel Wegkamp, Michael Meyer, Julia Stähler, and Martin Wolf — Fritz-Haber-Institut der MPG, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

Zinc oxide is a promising electrode material for organic optoelectronics, because of its large optical band gap, possible n-type conductivity and its abundance. Despite many years of research, the electronic structure of interfaces between ZnO and - possibly functional - molecules or even its vacuum interface are not well understood. We use femtosecond time- and angle-resolved two-photon photoemission spectroscopy (2PPE) to analyze both the occupied and *un*occupied electronic states and dynamics at such interfaces. We show that hydrogen adsorption, even for very low coverage, leads to the formation of a surface electron accumulation layer and thus surface metallicity. Above band gap excitation with 3.8 eV fs laser pulses leads to ultrafast relaxation of hot electrons in the ZnO$(10\bar{1}0)$ conduction band and the alleged formation of an excitonic state with a lifetime in the 100 ps range. Furthermore, we demonstrate that molecules with negative electron affinity allow for massive work function reduction of ZnO$(10\bar{1}0)$, e. g. by $\Delta\Phi = -2.9\,\mathrm{eV}$ in the case of a monolayer of pyridine. This opens a pathway to the design of cathodes with optimal electron injection barriers. We furthermore examine the changes in interfacial electronic structure upon biphenyl adsorption, which serves as a model system for optoelectronically functional poly(*p*-phenylene)-type molecules.

O 54.6 Wed 17:15 H33

Defect-Driven Interfacial Electronic Structure at a Hybrid Organic / Inorganic Heterojunction — •Oliver Monti[1], Leah Kelly[1], Laura Schirra[1], Paul Winget[2], Hong Li[2], and Jean-Luc Bredas[2] — [1]The University of Arizona, Tucson, AZ, USA — [2]Georgia Institute of Technology, Atlanta, GA, USA

We present a combined experimental and theoretical study of the interfacial electronic structure of highly defined thin films of organic semiconductors on ZnO. We discuss the importance of shallow donor states in the near-surface region of ZnO in determining energy-level alignment and electronic structure at such interfaces. Using ultraviolet and x-ray photoelectron spectroscopy together with two-photon photoemission and first-principles calculations we investigate the nature of hybrid interface states inside the bandgap of ZnO. These states display strong charge-transfer character and may play an important role in charge-harvesting events in organic photovoltaic cells.

O 54.7 Wed 17:30 H33

Electronic structure and excited states dynamics in polythiophene — •Lea Bogner[1], Gaurav Gupta[2], Michael Sommer[3], Mukundan Thelakkat[4], Thomas Thurn-Albrecht[2], and Petra Tegeder[1,5] — [1]Freie Universität Berlin, Fachbereich Physik — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik — [3]Albert-Ludwigs-Universität Freiburg, Institut für Makromolekulare Chemie — [4]Universität Bayreuth, Makromolekulare Chemie I — [5]Rubrecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut

Semiconducting conjugated polymers exhibit promising properties for applications in optoelectronic devices such as organic photovoltaic cells. Poly(3-hexylthiophene) (P3HT) and other poly- and oligothiophenes are auspicious electron donor materials due to their high charge carrier mobility. In this study thin films of semi crystalline P3HT with different degree of crystallinity [1] have been investigated by means of time- and angle-resolved two-photon photoemission (2PPE). We observed several unoccupied and occupied electronic states (bands) including the valence and conduction band. In addition two excited states are found which possess lifetimes in the order of hundred picoseconds.

Ref.: [1] Z. Wu, A. Petzold, T. Henze, T. Thurn-Albrecht, R. H. Lohwasser, M. Sommer, M. Thelakkat, Macromolecules, 2010, 43, 4646-4653.

O 54.8 Wed 17:45 H33

Charge transfer at the interface between substituted pentacene nanorods and gold single crystals — •Sabine-Antonia Savu, Maria Benedetta Casu, and Thomas Chassé — Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany

Pentacene is one of the most investigated organic molecules due to its successful application in organic electronics. Substitution in pentacene gives the opportunity to tailor the properties which are needed for applications; therefore it is necessary to investigate its influence on molecular aggregation and thin film formation. In particular, here we report our investigations on nanorods of three newly synthesized substituted pentacenes with different degrees of fluorination. We performed X-ray photoemission spectroscopy (XPS), near edge X-ray absorption fine structure (NEXAFS) spectroscopy, and atomic force microscopy (AFM) on nanorods deposited on Au(111) and Au(110) single crystals. XPS thickness dependent spectra in combination with NEXAFS investigations show that the screening of the core hole occurs via charge transfer from the metal to the molecule. In addition, the morphology of the nanorods has been investigated by using AFM, evaluating the nanorod characteristics also from a statistical point of view and taking the different degree of fluorination into account.

O 54.9 Wed 18:00 H33

Photoemission Investigation of the Electronic Structure of P3HT:PCBM Bulk-Heterojunctions using a lift-off technique — •Angela Eckstein[1,2], Dirk Hauschild[1,2], Julia Kern[3], Markus Mingebach[3], Carsten Deibel[3], Vladimir Dyakonov[3], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, 76021 Karlsruhe — [3]Experimentelle Physik VI, Universität Würzburg, 97074 Würzburg

Poly(3-hexylthiophene): phenyl-[6,6]-C61 butyric acid methyl ester (P3HT:PCBM) bulk heterojunctions (BHJ) are prototype active layers for organic solar cells. The electronic structure at the internal interface can be accessed by photoelectron spectroscopy (PES), thus providing insight into the alignment of the electronic levels and the occurrence of possible interface dipoles. However, the very surface sensitive PES investigation is complicated in case of P3HT:PCBM bulk heterojunctions since the film preparation by spin-coating creates a P3HT wetting layer on the film surface. In order to avoid this problem we used a lift-off technique to access the interface to the spin coating substrate (SiO2), which has shown to resemble the bulk situation [1]. P3HT:PCBM samples with different mixing ratio, which can be lift-off-prepared under UHV-condition thus avoiding contamination by ambient conditions, have been investigated by x-ray- and UV-PES as well as by inverse PES with particular respect to the influence of degradation and radiation damage. [1] Kahn et al. (Org. El. 11 (2010) 1779-1785)

O 54.10 Wed 18:15 H33

Bottom-up synthesis of self-aligned conjugated polymers — Sören Krotzky[1], •Rico Gutzler[1], Vijay Vyas[1,2], Bettina Lotsch[1,2], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Chemistry, University of Munich (LMU), Munich, Germany — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, Switzerland

We investigate the synthesis of self-assembled organometallic structures and well-defined long 1D polymers by the surface-supported Ullmann reaction on an Ag(111) surface. The brominated semiconducting precursor molecule (2,7-dibromobenzothieno[3,2-b]benzothiophene) is sublimed under UHV conditions on the crystalline surface where a dehalogenation step is induced at room temperature. STM reveals self-assembly of the dehalogenated ditopic molecule into short organometallic coordination polymers that arrange in a ladder-like monolayer. Annealing to 420 K leads to C-C coupling of the molecules via ejection of the coordinated metal atom. At this temperature the newly formed 1D polymer strands align in a side-by-side manner with three preferred directions with respect to the high-symmetry directions of the surface. DFT calculations show that the length of the synthesized polymers is sufficient to reduce the HOMO-LUMO gap to its value at infinite length of the polymer. Together with the calculated band-structure this suggests possible unidirectional charge mobility within the well-ordered semiconducting polymeric monolayer.

O 54.11 Wed 18:30 H33

How contact groups influence metal molecule hybrid structures under voltage — •Simon Liebing, Torsten Hahn, and Jens Kortus — TU Bergakademie Freiberg, Freiberg, Germany

In order to use molecules in electronics it is not only important to understand the properties of molecules themself but also properties of metal-molecule interfaces. Recent contributions discussed the behavior of thiole [1] and amino linker groups [2]. To get a more systematic understanding the authors have chosen a model system of benzene with variable linker groups between gold electrodes. Such groups can be thiole, amino, thiophen, nitrile, pyrol and cyanide. This allows for example to study the differences between σ- and π- like symmetry with respect to the individual interface geometry. The theoretical study combines the calculation of single molecule properties by density functional theory [3] with the nonequilibrium Greens functions technique [4] to calculate the transport properties [5] of the device. [1] Markussen, T. et al. JCP **132** , 224104 (2010)

[2] Angela, D. et. al. Nano Letters **10**, no. 7 (2010)
[3] Pederson, M. et. al. Phys. Status Solidi b **217**, 197. (2000)
[4] Datta, S. Nanotechnology **15**, 433. (2004)
[5] Brandbyge, M. Phys. Rev. B **65**, 165401 (2002)

O 54.12 Wed 18:45 H33

Improving the contact materials of organic electronic devices: Polymeric dipole layers vs. self assembling monolayers — •Janusz Schinke[1,2], Julian Heusser[3,2], Marc Hänsel[3,2], Julia Maibach[4,2], Wolgang Kowalsky[1,2], Michael Kröger[1,2], Eric Mankel[4,2], and Wolfram Jaegermann[4,2] — [1]TU Braunschweig, Institut für Hochfrequenztechnik — [2]Innovation Lab GmbH — [3]Universität Heidelberg, Kirchhoff-Institut für Physik — [4]TU Darmstadt, Materials Science Institute, Surface Science Division

In organic electronic devices, charge injection at the contacts is crucial for high electrical performance. Most of these devices require at least one electrode with a sufficiently low work function (WF). Low-WF electrodes like alkaline earth metals are easily available; however, they are chemically very reactive and oxidize in ambient atmosphere. A smart way to overcome this problem is the use of molecular or polymeric dipole layers (PDLs). The use of PDLs to tune an electrodes work function can be advantageous over self assembled monolayers(SAMs) as the PDL concept can be applied to a wider range of electrode materials like ITO, Ag, Au or Al. We have used two different PDLs: branched polyethylenimine (PEI) and polyethyleneimine ethoxylate (PEIE). We studied the the properties of PDL treated substrates via AFM, ambient Kelvin probe and XPS/UPS. Both interlayers lower the metal substrate work function by approx. 1000meV. On ITO we reach absolute values of about 3.0eV which leads to strongly enhanced electron injection in model devices.

O 55: Electronic Structure and Spin-Orbit Interaction II

Time: Wednesday 16:00–19:15 Location: H42

O 55.1 Wed 16:00 H42

Hexagonal warping effects in the spin-split electronic structure of the BiAg$_2$ surface alloy — •Hendrik Bentmann[1,2], Mattia Mulazzi[1,2], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg, Germany — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe, Germany

Whereas the Rashba-model predicts an isotropic spin-orbit (SO) splitting and an in-plane spin orientation for the electronic states in a two-dimensional electron gas (2DEG), the anisotropic lattice symmetries in a real system can lead to significant deviations from this scenario. Based on angle-resolved photoemission experiments, we discuss such effects for the surface states of the BiAg$_2$ surface alloy, a prototype model system for SO effects in 2DEGs. The dispersion of the surface states shows a pronounced hexagonal warping which is accurately captured by $k\cdot p$-theory taking into account the C_{3v}-symmetry of the surface. Additionally, we find threefold modulations in the photoemission intensity giving hints on the influence of the lattice symmetry on the orbital character of the electronic states. We compare our results on BiAg$_2$ with similar effects in the surface electronic structure of the topological insulator Bi$_2$Te$_3$(0001).

O 55.2 Wed 16:15 H42

Single Dirac-cone on the Cs-covered topological insulator surface Sb$_2$Te$_3$(0001) — •Christoph Seibel[1,2], Hendrik Bentmann[1,2], Henriette Maass[1,2], Sebastian Fiedler[1,2], Christian Junger[1,2], Chul-Hee Min[1,2], Kazuyuki Sakamoto[3], Friedrich Reinert[1,2], and Kenya Shimada[4] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe — [3]Graduate School of Advanced Integration Science, Chiba University, Chiba 263-8522, Japan — [4]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

In contrast to more prominent topological insulator (TI) materials like Bi$_2$Te$_3$ and Bi$_2$Se$_3$ the surface electronic structure of naturally p-type Sb$_2$Te$_3$ is comparably unexplored. Using angle-resolved photoelectron spectroscopy (ARPES) we measured the occupied electronic structure of clean and Cs-covered Sb$_2$Te$_3$(0001). The surface-doping-induced band bending results in a non-rigid shift of the electronic valence band features leaving the Dirac-point right above the Fermi-level. The influence of the adatoms is compared to effects of metal adsorption on other TI surfaces. Furthermore we identify a trivial, Rashba-split surface state by photon-energy-dependent ARPES and studied its spin-character using spin-resolved ARPES.

O 55.3 Wed 16:30 H42

Determining the Rashba splitting of BiCu$_2$/Cu(111) by STS via interband scattering — •Manuel Steinbrecher[1], Hasmik Harutyunyan[1], Christian R. Ast[2], and Daniel Wegner[1] — [1]Physikalisches Institut and CeNTech, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Max Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

Rashba systems are a promising class of materials for use in spintronics applications. They are characterized by surface states that are spin-split in k-space due to strong spin-orbit coupling. Well-known Rashba systems under recent investigation are alloys on noble metal surfaces. We have examined one of these surface alloys, Bi/Cu(111), by STM and STS measurements. By evaluating standing waves of the Rashba-split surface states, we have expanded an elegant method for measuring surface-state dispersions and compared the results with ARPES measurements and DFT calculations. For occupied states, we have found multiple intra- and interband scattering channels that enable the quantitative determination of band dispersions including the Rashba splitting. The results are in very good agreement with ARPES data and demonstrate the usefulness of this strategy to determine the band structure of Rashba systems. The lack of possible scattering channels will be discussed in terms of spin polarization and hybridization effects. We will provide an outlook on results regarding unoccupied states where DFT predictions mostly lack experimental verification.

O 55.4 Wed 16:45 H42

Theory of spin-orbit coupling at LaAlO3/SrTiO3 interfaces and SrTiO3 surfaces — •Zhicheng Zhong — Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria

The theoretical understanding of the spin-orbit coupling (SOC) effects at $LaAlO_3/SrTiO_3$ interfaces and $SrTiO_3$ surfaces is still in its infancy. We perform first-principles density-functional-theory calculations and derive from these a simple tight-binding Hamiltonian, through a Wannier function projection and group theoretical analysis. We find striking differences to the standard Rashba theory for spin-orbit coupling in semiconductor heterostructures due to multi-orbital effects: by far the biggest SOC effect is at the crossing point of the xy and yz (or zx) orbitals; and around the Γ point a Rashba spin splitting with a cubic dependence on the wave vector $\vec{k}$ is possible.

O 55.5 Wed 17:00 H42

Strong correlations at topological insulator surfaces and the breakdown of the bulk-boundary correspondence — •Manuel Schmidt — RWTH Aachen, Deutschland

The criteria for strong correlations on surfaces of three-dimensional topological insulators are discussed. Usually, the Coulomb repulsion at such surfaces is too weak for driving a phase transition to a strongly correlated regime. I discuss a mechanism and possibilities of its experimental implementation by which the strength of the Coulomb interaction can be tuned over a wide range. In the strongly interacting regime, the surface states are gapped, even though the topological classification of the bulk band structure predicts gapless surface states.

O 55.6 Wed 17:15 H42

Bi/Ag(111) - A "Bird's Eye View" - Spin-resolved Band Structure above the Fermi Level — •Sune N. P. Wissing[1], Anke B. Schmidt[1], Fabian Zinser[2], Klaus Kern[2], Christian R. Ast[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Max-Planck-Institut für Festkörperforschung Stuttgart, Germany

We studied the unoccupied electronic structure of the surface alloy Bi/Ag(111) $(\sqrt{3}\times\sqrt{3})\,R30^\circ$ with scanning tunneling spectroscopy and spin- and angle-resolved inverse photoemission. The adsorption of heavy elements on noble-metal surfaces results in surface alloys, which exhibit surface states with large Rashba-type spin splittings. Detailed information about the occupied electronic structure is available from various angle-resolved photoemission studies. Above the Fermi level, we have identified several unoccupied states with significant spin dependence. We determined their nature regarding symmetry and bulk vs. surface character as well as their energy vs. momentum dispersion and their spin dependence. We will discuss our results in the light of theoretical calculations [1].

[1] G. Bihlmayer *et al.*, PRB **75**, 195414 (2007)

O 55.7 Wed 17:30 H42

Rashba-Type Spin-Split Surface: $(\sqrt{3}\times\sqrt{3})$Bi/Ag(111)$R30^\circ$ — •Lydia El-Kareh, Paolo Sessi, Thomas Bathon, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We report on low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS) investigations of the $(\sqrt{3}\times\sqrt{3})$Bi/Ag(111)$R30^\circ$ surface alloy, that has been reported to show a giant Rashba-Bychkov (RB) effect [1,2]. Comparison of our STS data with photoemission experiments and first principle calculations [3] allow the identification of two downward dispersing spin-split surface states with onsets at −100 meV and +725 meV with respect to the Fermi level. Bias-dependent quasi-particle interference maps reveal a striking energy dependence of scattering processes at step edges and around impurities. Based on a detailed analysis of the obtained data we will discuss the band dispersion and spin topology of both bands.

[1] C. R. Ast *et al.*, Phys. Rev. Lett. **98**, 186807 (2007).
[2] C. R. Ast *et al.*, Phys. Rev. B **75**, 201401(R) (2007).
[3] G. Bihlmayer *et al.*, Phys. Rev. B **75**, 195414 (2007).

O 55.8 Wed 17:45 H42

Unoccupied surface state of Tl/Si(111): Rotating spin and giant splitting — •Sebastian D. Stolwijk[1], Kazuyuki Sakamoto[2], Anke B. Schmidt[1], Peter Krüger[3], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster — [2]Graduate School of Advanced Integration Science, Chiba University, Japan — [3]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster

Spin-resolved inverse photoemission experiments reveal the unoccupied electronic structure along the $\bar{\Gamma}\bar{\mathrm{K}}$ direction of the Tl/Si(111)-(1×1) surface. Our recently developed **RO**tatable **S**pin-polarized **E**lectron source (ROSE) enables measurements of the in-plane and out-of-plane component of the polarization vector. With this, we identify a spin-orbit split surface state, whose polarization vector rotates from the usual Rashba direction to the direction perpendicular to the surface upon approaching the $\bar{\mathrm{K}}$ point. This effect can be simply understood as a consequence of the 2D symmetry of the hexagonal system [1]. Remarkably, the spin-orbit split surface state shows almost complete out-of-plane polarization with opposing sign at the $\bar{\mathrm{K}}$ and $\bar{\mathrm{K}}'$ point. Moreover, the spin-orbit split surface state exhibits a giant splitting in energy of more than 0.5 eV. Our results are supported and discussed on the basis of calculations within the GW approximation including spin-orbit coupling. Charge distributions of the surface state reveal that the giant splitting is due to a strong localization close to the Tl atom.

[1] K. Sakamoto et al., Phys. Rev. Lett. **102**, 096805 (2009)

O 55.9 Wed 18:00 H42

Origin of Rashba-splitting in the quantized subbands at the Bi_2Se_3 surface — •Hadj Mohamed Benia[1], Alexander Yaresko[1], Andreas P. Schnyder[1], Jürgen Henk[2], Chengtiang Lin[1], Klaus Kern[1,3], and Christian R. Ast[1] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]Institut für Physik -Theoretische Physik, Martin-Luther-Universität Halle-Wittenberg, D- 06099 Halle (Saale), Germany — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

We study the band structure of the Bi_2Se_3 topological insulator (111) surface using angle-resolved photoemission spectroscopy (ARPES). We examine the situation where two sets of quantized subbands exhibiting different Rashba spin-splitting are created via bending of the conduction (CB) and the valence (VB) bands at the surface. We show that the potential gradients at both 2DEGs are similar and therefore not responsible for the splitting discrepancy. On the other hand, first principles calculations show that the contribution of Bi 6p states to the VB is clearly smaller than to the CB. Therefore, and since Bi 6p states are characterized by a strong spin-orbit coupling (SOC), the spin-splitting discrepancy is traced back to a difference in the SOC strength.

O 55.10 Wed 18:15 H42

Visualizing Anderson Localization of Non-Interacting Electrons — Fabian Zinser[1], Maurits W. Haverkort[1], Sune N. P. Wissing[2], Anke B. Schmidt[2], Markus Donath[2], Klaus Kern[1], and •Christian R. Ast[1] — [1]MPI für Festkörperforschung, 70569 Stuttgart — [2]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

Randomness destroys translational invariance resulting in exponential spatial localization of wave functions through quantum interference. This effect — known as Anderson localization — is a universal property of waves, which has been observed directly in light and matter. In electron systems, Anderson localization has been studied mostly indirectly in transport experiments through metal-insulator transitions or conductance fluctuations. This complicates theoretical descriptions as, e. g., calculating the conductance remains a challenging task despite highly sophisticated models. Using the Bi_xPb_{1-x}/Ag(111) mixed surface alloy, we go beyond averaged quantities both in theory and experiment. We measure simultaneously chemical composition and local electronic structure linking experiment and theory on the most fundamental level: we demonstrate the atomically resolved observation of spatial wave function localization for a mixed surface alloy — a purely two-dimensional electron system in a static disordered potential. We then use the chemical composition as the structural input for the "original" real space Anderson tight-binding model which allows us to directly compare the locally resolved wave functions in experiment and theory with remarkable agreement.

O 55.11 Wed 18:30 H42

Spin Polarized Photoemission from Bi2Te3 and Sb2Te3 Topological Insulator Thin Films — •Lukasz Plucinski[1,2], Alexei Herdt[1,2], Gustav Bihlmayer[3], Gregor Mussler[4], Sven Döring[2], Detlev Grützmacher[4], Stefan Blügel[3], and Claus M. Schneider[1,2] — [1]Peter Grünberg Institute PGI-6, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [3]Peter Grünberg Institute PGI-1, Forschungszentrum Jülich, 52428 Jülich, Germany — [4]Peter Grünberg Institute PGI-9, Forschungszentrum Jülich, 52428 Jülich, Germany

Spin polarized photoemission spectra from surfaces of Bi2Te3 and Sb2Te3 thin films show up to 45% in-plane spin polarization in the Dirac cone near the Fermi level, which is consistent with the dedicated ab initio theoretical results which find spin polarization in the order of 40-50% when averaged over the surface quintuple layer with the exponential depth profile related to the scattering mean free path of the VUV photoelectrons. Furthermore a non-zero out-of-plane spin polarization component is found in the Bi2Te3 hexagram Fermi surface.

We will discuss the spin-orbit entanglement mechanism behind the non-100% spin polarization in topologically protected surface states, and propose possible surface engineering solutions to increase the spin polarization of the Dirac cone in films grown by the MBE. Furthermore we will compare analytical band structure models with the DFT-based slab calculations.

O 55.12 Wed 18:45 H42

Electron dynamics of the topological insulator Bi_2Te_2Se — •Daniel Niesner[1], Thomas Fauster[1], Oleg Tereshchenko[2,4], Konstantin Kokh[3,4], and Evgueni Chulkov[5] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 A3, 91058 Erlangen — [2]Institute of Semiconductor Physics, 630090 Novosibirsk, Russia — [3]Institute of Geology and Mineralogy, 630090 Novosibirsk, Russia — [4]Tomsk State University, 634050 Tomsk, Russia — [5]Donostia International Physics Center (DIPC), 20018 San Sebastián/Donostia, Basque Country, Spain

In addition to the conventional Dirac cone, bismuth chalcogenides exhibit a high-lying topological surface state (TSS) in a projected bulk bandgap 1...1.5 eV above the Fermi level [1].

Bichromatic two-photon photoemission (2PPE, $h\nu = 1.65\,\text{eV} + 4.65\,\text{eV}$) was employed to follow the transient occupation of this state and the conduction band (CB*) above it. In addition, an image-potential state (IPS) is observed at a similar final-state energy. From a careful analysis of the polarization- and the time-dependence of the 2PPE data, the lifetimes of the single states are deconvolved. They amount to 25 fs (IPS), 22 fs (TSS) and 13 fs (CB*). Also, a linear energy-dependence of the decay rate of the conduction band below the TSS is found, as it is characteristic for layered materials [2].

[1] D. Niesner *et al.*, Phys. Rev. B 86, 205403 (2012)
[2] S. Xu *et al.*, Phys. Rev. Lett. 76, 483 (1996)

O 55.13 Wed 19:00 H42

Computing the LDOS for a disordered 2DEG with Rashba-type spin orbit interaction — Jascha Ulrich[1], Serge Florens[2], •Markus Morgenstern[1], Daniel Hernangomez[3], and Thierry Champel[3] — [1]2. Physikalisches Institut B, RWTH Aachen — [2]Institut Néel, CNRS/UJF, Grenoble — [3]LPMMC, CNRS/UJF, Grenoble

We present the application of a recent formalism developed by Serge Florens and Thierry Champel for the description of the single-electron dynamics under high magnetic fields in smoothly varying potential landscapes to systems with Rashba-type spin-orbit interaction subject to disorder both in the electrostatic potential $V(\vec{r})$ and the Rashba parameter $\alpha(\vec{r})$. Assuming an electrostatic disorder potential $V(\vec{r})$ and a Rashba parameter $\alpha(\vec{r})$ in the plane of the two-dimensional electron gas which vary locally linear on the scale of the magnetic length l_B and working in the high-field limit of negligible Landau level mixing, we present a compact formula for the temperature-broadened local density of states $\rho^{\text{STS}}(\omega, \vec{r})$ as measured in an STS experiment according to the popular Tersoff-Hamann formula for setups with constant tip density of states. The resulting expression can efficiently be evaluated numerically by Fourier transform methods on home computers for arbitrary electrostatic and Rashba disorder maps. Explicit analytic expressions for limiting cases of zero temperature and constant Rashba parameter are given. We discuss the effects of the electrostatic potential and Rashba fluctuations on the electron dynamics and the form of the local density of states.

O 56: Oxide Surfaces I

Time: Wednesday 16:00–19:00 Location: H45

O 56.1 Wed 16:00 H45

scanning tunneling microscopy study of single-crystalline Sr3Ru2O7 — •Bernhard Stöger[1], Zhiming Wang[1], Marcel Hieckel[1], Florian Mittendorfer[1], Raimund Podloucky[2], Josef Redinger[1], David Fobes[3], Zhiqiang Mao[3], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institute of Applied Physics, Vienna University of Technology, Vienna, Austria — [2]Institute for Physical Chemistry, University of Vienna, Austria — [3]Department of Physics and Engineering Physics, Tulane University, New Orleans, LA, USA

Investigating surface defects such as oxygen vacancies and the adsorption of relevant molecules helps gaining more insight into the physics behind solid oxide fuel cells and catalytic processes.

High-quality $Sr_3Ru_2O_7$ (SRO) single crystals were grown using the floating zone technique. The SRO samples were cleaved at 100 K under UHV conditions and subsequently investigated by STM at 78 K and 6 K. To determine which species are imaged in STM, doped SRO samples were investigated and STM simulations were performed. Furthermore, we have characterized the defects that are present at the as-cleaved surfaces, and how reactive they are if exposed to CO, O2 and CO2.

CO adsorbs on the perfect surface at the position of the apical oxygen atom. The adsorbed CO can be easily manipulated by the STM tip. At +1 V a reaction takes place which changes the appearance of the adsorbed CO drastically. At +2.7 V the CO molecules start to diffuse on the surface and to desorb. This work was supported by the Austrian Science Fund (FWF project F45).

O 56.2 Wed 16:15 H45

Reversible transitions between surface reconstructions on SrTiO3 — •Stefan Gerhold, Zhiming Wang, Xianfeng Hao, Michael Schmid, and Ulrike Diebold — Institute of Applied Physics, TU Wien, Austria

$SrTiO_3$ as an archetypical perovskite oxide has attracted intense interest in diverse fields ranging from fundamental solid-state physics and chemistry, materials science to electronics applications. In all these applications, the surface properties are of vital importance. We study the evolution of surface reconstructions on the $SrTiO_3(110)$ and (001) surface using STM, LEED, XPS and ISS. Atomically well-defined $SrTiO_3(110)$ surfaces can be obtained by Ar^+ sputtering and annealing. Mono-phased reconstructions are obtained, and can be transformed into each other reversibly by depositing Sr or Ti followed by annealing. The most commonly-observed $SrTiO_3(110)$ (4×1) reconstruction consists of a layer of TiO_4 tetrahedra, which forms a network of six- and ten-membered rings by corner-sharing oxygen atoms. The mirror symmetry in the six-membered rings is broken along the [1-10] direction, therefore two degenerate anti-parallel (4×1) domains are formed. Two types of vacancies are present at domain boundaries. These can be tuned by adjusting the oxygen pressure during annealing; depending on the type of domain boundary different band bending is observed. At the $SrTiO_3(001)$ surface a reversible change between $c(4 \times 2)$, (2×2), (1×1), and $c(2 \times 2)$ reconstructions can also be achieved by evaporating Sr or Ti followed by annealing. This work was supported by the Austrian Science Fund (project F45).

O 56.3 Wed 16:30 H45

Reversible transformation between α-Fe_2O_3 and Fe_3O_4 — •Francesca Genuzio, Alessandro Sala, Thomas Schmidt, and Hans-Joachim Freund — Fritz-Haber-Institut, Abt. CP, 14195 Berlin

The characterization of the properties of iron oxide thin films and their surfaces is a promising research field, considering the variety of applications those materials are interesting for. The peculiarity of this class of oxides is to assume different properties according to their crystal structure, defined both by stoichiometry and preparation. In thin films, in particular, the influence of the substrate on the quality of the supported oxide-surface and on its thermodynamics is still not clear; moreover the phase diagram of these systems can differentiate significantly from that calculated for bulk materials. We present a combined LEEM and LEED study focused on the systematic characterization of the conditions to reversibly transform α-Fe_2O_3 and Fe_3O_4 thin films on Pt(111) and on Ag(111). Experiments were carried out with the SMART spectro-microscope, an aberration-corrected energy-filtered LEEM-PEEM system which allows the observation in real time and in situ of the surface with high acquisition rate. A complete characterization of oxidation and reduction of mixed-phase films, as well as the substrate role in such reactions, is discussed.

O 56.4 Wed 16:45 H45

Growth of ultrathin samaria films on Pt(111) studied by LEED and STM — •J.H. Jhang[1], A. Schaefer[1], W. Cartas[2], J.F. Weaver[2], and M. Bäumer[1] — [1]Institute for Applied and Physical Chemistry, University of Bremen, Germany — [2]Department of Chemical Engineering, University of Florida, USA

Samaria has been considered as a highly selective catalyst for oxidative coupling of methane (OCM). It also exhibits catalytic activity for dehydration reactions, e.g. the decomposition of 2-propanol. Heterocatalytic reactions take place on the surface of catalysts, thus the selectivity and activity of oxide catalysts strongly depend on surface defects, surface structures, and also oxygen storage and release capabilities. While other rare earth oxides like ceria have been studied intensively, detailed surface science studies on samaria are still lacking. In this contribution we report an investigation of ultrathin samaria films grown on a Pt(111) substrate. Samaria films were prepared by physical vapor deposition (PVD) of Sm metal in O_2 ($p = 5 \times 10^{-7}$ mbar) at 600 K substrate temperature, then post-annealed in O_2 at 1000 K in order to obtain well-ordered samaria structures. The well-ordered structures have been characterized via low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). Both LEED and STM results reveal a lattice parameter of the samaria films close to the (111) surface orientation of C-type Sm_2O_3. Annealing treatments in UHV caused significant topographic changes to the films, accompanied by the formation of a cubic phase in (001) orientation, most likely SmO, due to partial reduction.

O 56.5 Wed 17:00 H45

Dynamic behavior of anti-phase boundaries in the layer-by-layer growth of Fe_3O_4(111)/Pt(111) thin films — Alessandro Sala, Helder Marchetto, •Thomas Schmidt, and Hans-Joachim Freund — Fritz-Haber-Institut, Abt. CP, 14195 Berlin

The transition-metal oxide Fe_3O_4 (magnetite) has a wide range of applications in heterogeneous catalysis and magnetism. The kind of preparation influences the film properties; in particular, anti-phase boundaries, i.e. dislocations and rotational domain boundaries, play an active role for the anomalous film resistivity and magnetic susceptibility, and could be a considerable factor in the determination of surface electronic properties. A new preparation recipe has been applied to study in-situ and in-real-time the layer-by-layer growth of a complete Fe_3O_4(111) film on Pt(111) with the SMART, the aberration-corrected energy-filtered LEEM/PEEM installed at BESSY II in Berlin. In addition to the usual atomic steps, the oxide surface shows new line defects, which can be interpreted as line dislocations. Furthermore, dark field imaging of the Fe_3O_4 surface visualize domains rotated by 180° against each other. The formation of the dislocations and the rotations domains and their behavior during growth and annealing are discussed.

O 56.6 Wed 17:15 H45

A first-principles view of the Cabrera-Mott Model of Metal Oxidation — •Anders Hellman, Jakub Baran, and Henrik Grönbeck — Chalmers, Applied Physics, Göteborg, Sweden

Oxidation of metals is an every-day phenomenon, which can be an unwanted process, e.g., automotive corrosion. However, under controlled conditions oxidation is of enormous practical importance, both in industry and science. The work of Cabrera and Mott (CM) in the mid-twenty century still remains the main theoretical model for growth of thin oxides on metals [1]. Recently, Zhou et al. [2] have experimentally shown that the limiting thickness of the aluminum oxide on Al(111) can be tuned by the oxygen pressure. Our first-principles calculations [3] support many of the key assumptions of the CM model. For instance, based on our results we estimated the limiting thickness of Al2O3 on Al(111) to around 16 Å, which agrees well with the experimental data. Furthermore, the charge transfer to adsorbed oxygen molecules generates a Mott potential which value also agrees well with experimental estimates. However, the underlying reason for observing a limiting thickness of the protective oxide is not the diminishing effect of the Mott potential. Instead we will provide another underlying reason for the limiting thickness based on our first-principles calculations.

References 1.*Cabrera, N. and N.F. Mott, Reports on Progress in Physics 12 163 (1948). 2.*Cai, N., et al., Phys. Rev. Lett. 107 035502 (2011). 3.*Baran, J., Grönbeck, H., Hellman, A., submitted

O 56.7 Wed 17:30 H45

Adsorption of Fe on Fe_3O_4(111) surfaces — Tomasz Pabisiak and •Adam Kiejna — University of Wroclaw, Institute of Experimental Physics, Poland

Iron oxides are abundant and important in many geochemical and environmental processes, and technological applications. The chemical reactivity of the oxide surface can be significantly modified by deposition of various species that leads to catalytic activity of such complex. We applied the spin-polarized density functional theory (DFT) and the DFT+U method, accounting for the effect of strong on-site Coulomb correlations, to study the submonolayer adsorption of Fe atoms on magnetite (111) surfaces. Adsorption on two stable terminations has been studied: one terminated with iron and the other with oxygen. We have found that the presence of Fe adatom induces large changes in the geometry of magnetite surface. Fe binds strongly to magnetite and the bonding to the O-terminated surface is distinctly stronger than that to the Fe-termination. Structural, electronic and magnetic properties of magnetite surface covered with iron and noble metals [1] are compared and discussed. Similarly as for clean magnetite surface, upon Fe adsorption DFT and DFT+U provide qualitatively similar surface geometries but they differ substantially in the prediction of the surface energetics.

[1] A. Kiejna, T. Ossowski, T. Pabisiak, Physical Review B 85 (2012) 125414.

O 56.8 Wed 17:45 H45

CO Induced Adatom Sintering in a Model Catalyst: Pd/Fe3O4 — •Zbynek Novotny[1], Gareth S. Parkinson[1], Giacomo Argentero[1], Michael Schmid[1], Jiri Pavelec[1], Rukan Kosak[2], Peter Blaha[2], and Ulrike Diebold[1] — [1]Institute of Applied Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10/134, 1040 Vienna, Austria — [2]Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, 1060 Vienna

The coarsening of catalytically-active metal clusters is often accelerated by the presence of gases through the formation of mobile intermediates. We use scanning tunneling microscopy (STM) to follow the CO induced coalescence of Pd adatoms supported on the Fe3O4(001) surface at room temperature. Pd-carbonyl species, formed via the so-called 'skyhook' effect, are responsible for Pd mobility in the system. Using time-lapse STM, key steps of cluster nucleation and growth are observed in an atom-by-atom fashion.

This material is based upon work supported as part of the Centre for Atomic-Level Catalyst Design, an Energy Frontier Research Centre funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number #DE-SC0001058.

O 56.9 Wed 18:00 H45

Water adsorption on ultra-thin ZrO_2/Pt_3Zr — •joong il jake choi, hao li, christian weilach, ulrike diebold, and michael schmid — Technische Universität Wien, Wien, Austria

Despite its importance in many areas of industry such as catalysis, fuel cell technology and microelectronics, the surface properties of ZrO_2 are yet not well understood. We have prepared ultra-thin ZrO_2 films by oxidation of a Pt_3Zr(0001) crystal [1] and studied adsorption and desorption of water on this surface by STM, XPS and AES. Water on ZrO_2/Pt_3Zr(0001) appears as a bright species on STM. Adsorption strongly depends on the structure of the substrate below the oxide; the lowest coverage is found in areas with unreconstructed Pt(111) below the oxide. Depending on the predominant substrate structures, we find a saturation coverage at room temperature between 0.14 and ≈ 0.25 ML with respect to the oxide lattice. The water species are adsorbed on equivalent sites of the oxide lattice, often also in equivalent sites with respect to the alloy substrate, thus influenced by the superstructure lattice (moiré). XPS suggests that the species observed by STM are the hydroxyl group. We have also created stable oxygen vacancies by electron irradiation of the ZrO_2 film and studied the adsorption of H_2O on this surface with defects.

[1] M. Antlanger et. al., Phys. Rev. B 86, 035451 (2012)

O 56.10 Wed 18:15 H45

Adsorbed water structures on alkaline earth metal oxide (001) surfaces at realistic conditions: A first-principles study — •Xunhua Zhao, Eric Huynh, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem 14195, Germany

Understanding the interaction between water and oxide surfaces is of fundamental importance for basic and engineering sciences. Recently, one-dimensional structures have been observed on CaO(001) in the presence of H_2O [1]. Such structures have not been reported so far for MgO and SrO. We performed a free-energy-based *ab initio* genetic algorithm and atomistic thermodynamics analysis to find stable structures of water adsorbed on MgO(001), CaO(001) and SrO(001). The structures were searched without stoichiometric constraints. Density-functional theory with semilocal (PBE) and hybrid (HSE06) exchange-correlation functionals with a first-principles dispersion interaction correction was employed. Our results confirm the presence of a range of H_2O chemical potentials around the experimental conditions (T = 300 K, p_{H_2O} = 10^{-9} atm) where one-dimensional adsorbed water structures are preferred on CaO(001). Trends in the range of stability and conditions for one-dimensional versus monolayer structures on MgO(001), CaO(001), and SrO(001) will be discussed and related to differences in the electronic structure of the oxides. The accuracy of the functionals is analyzed based on the "exact-exchange plus correlation in the random-phase approximation" approach.—[1] X. Shao, N. Nilius, M. Sterrer, Y. Fujimori, and H.-J. Freund, to be published.

O 56.11 Wed 18:30 H45

DFT calculations of surface properties of Li_2FeSiO_4 — •Nicolas Hörmann[1,2] and Axel Gross[1,2] — [1]Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, Albert-Einstein-Allee 11, 89069 Ulm — [2]Universität Ulm, Institut für Theoretische Chemie, Albert-Einstein-Allee 11, 89069 Ulm

Li_2FeSiO_4 is a promising new electrode material for Lithium ion batteries, due to the abundance, low cost and safety of the elemental components and the high theoretical energy densities of up to 300 mAh/g [1]. Though rarely studied, surface properties can be decisive for electrode performance in Li ion batteries [2].

Electronic structure calculations based on density functional theory (DFT) have been performed for different surface terminations of Li_2FeSiO_4 to determine the influence of surface properties on relevant electrode parameters. In particular, surface energies of stable surfaces and thus equilibrium crystallite morphologies are determined for different chemical environments, surface compositions and crystal structures. Furthermore, models are presented that allow the estimation of surface energies from bulk properties prior to time consuming ab-initio calculations. The applicability and range of validity of the models is analysed and discussed.

[1] M. Saiful Islam et al. , *J. Mater. Chem.*, **2011**, *21*, 9811.
[2] Kyu-Sung Park et al., *Chem. Mater.*, **2012**, *24 (16)*, pp 3212–3218.

O 56.12 Wed 18:45 H45

Ab initio study of low-coordinated sites on MgO(100) using hybrid functionals — •Philipp Auburger[1], Manuel Kolb[1,2], and Michel Bockstedte[1] — [1]Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]Leiden Institute of Chemistry, Leiden University, Leiden, Netherlands

Low-coordinated surface sites, such as surface oxygen vacancies and step edges are reactive centers at the MgO(100) surface. To unravel their role in chemical reactions and as optical recombination centers, it is pivotal to understand their electronic states. Density functional theory together with the (semi-)local exchange-correlation functionals, however, underestimate the band gap of metal oxides by a large margin. Hybrid functionals like the HSE06, are known[1] to improve the description of metal oxides considerably. Here we investigate surface color centers on the MgO(100) surface including the step edges, oxygen vacancy on the surface and at step edges, as well as kink sites using the DFT-HSE06 approach and a slab model. This enables a proper description of defect and dispersing shallow step edge states. For both states we find large corrections to values obtained with standard functionals. In addition, the calculations reveal a negative electron affinity in agreement with GW calculations.[2] We compare our results with recent STS-experiments on color centers at MgO-films.[3]

[1] G. Pacchioni, J. Chem. Phys. 128, 182505 (2008).
[2] M. Rohlfing , et al, Phys. Rev. Lett. 91, 2568021 (2003).
[3] M. Sterrer et al, J Phys. Chem.B 110, 46-49 (2006).

O 57: Graphene: SiC Substrates and Intercalation (jointly with HL, MA and TT)

Time: Wednesday 16:00–19:15 Location: H17

O 57.1 Wed 16:00 H17

Molecular Doping of Epitaxial Graphene on SiC with flouro-fullerenes — •Martina Wanke[1,2], Anton Tadich[3], Mark Edmonds[4], Yaou Smets[4], Chris Pakes[4], and Thomas Seyller[1,2] — [1]Institut für Physik, Technische Universität Chemnitz, Reichenhainer Strasse 70, 09126 Chemnitz, Germany — [2]LS Technische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erwin-Rommel-Strasse 1, 91058 Erlangen — [3]Soft-X-Ray-Beamline, Australian Synchrotron, 800 Blackburn Road, Clayton, VIC 3168, Australia — [4]Scholl of Physics, La Trobe University, Physical Sciences 1, Bundoora, VIC 3086, Australia

Epitaxial graphene (EG) on SiC(0001) is intrinsically n-type doped due to charge transfer from the substrate surface [1,2]. Charge transfer doping with F4-TCNQ reduces the carrier concentration and increases the carrier mobility [2], but the stability of the molecular layer in ambient conditions is not given [2]. Molecules with a sufficiently high electron affinity are needed in order to achieve a significant reduction of the electron concentration in EG by surface transfer doping. The mechanism of surface transfer doping of diamond with $C_{60}F_{48}$ is well understood [3]. Using ARPES we investigated the surface transfer doping of EG with $C_{60}F_{48}$. A net p-type doping of EG was observed for higher coverages of the $C_{60}F_{48}$.

[1] T.Ohta et al., Science **313** (2006) 951; [2] J.Jobst et al., PRB **81** (2010) 195434; W.Chen et al., JACS **129** (2007) 10418; C. Coletti et al., PRB **81** (2010) 235401. [3] M. T. Edmonds et al., JCP 136 (2012) 124701.

O 57.2 Wed 16:15 H17

Transport properties of epitaxially grown graphene nanostructures — •Jens Baringhaus, Frederik Edler, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The patterning of graphene into small stripes, the so called graphene nanoribbons, is an essential task for the development of future graphene based electronic devices. For such ribbons with a well-ordered edge geometry the presence of one-dimensional edge states has been predicted. The fabrication of these well-defined structures requires the avoidance of any damaging post-processing. To overcome this obstacle we use a selective graphitization process on SiC-mesa structures, producing monolayer graphene nanoribbons of 40 nm to 100 nm in width and of several micrometers in length. The local electronic properties of the ribbons are investigated by means of a 4-tip STM. The self-assembled graphene nanoribbbons show metallic behavior and can be clearly distinguished from the non-metallic substrate. Conductances close to $G_0 = e^2/h$ are observed for a wide temperature range from 30 K up to room temperature. Description within the Landauer formalism is possible assuming ballistic transport dominated by a single ballistic channel. This is a strong indication for spin-polarized transport through the edge-states of the ribbons. These edge states also show up in scanning tunneling spectra. At higher temperatures the conductance increases due to the occupation of the next subband. Remarkably all investigated ribbons exhibit very large mean free paths up to 15 μm.

O 57.3 Wed 16:30 H17

Local investigation of transport properties and morphology of epitaxially grown 2d graphene — •Frederik Edler, Jens

Baringhaus, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

Graphene has a peculiar band structure and special transport properties. The transport is strongly affected by imperfections of the graphene films, e.g atomic steps and impurities located at the interface between graphene and its support. A reliable control of these parameters is possible by epitaxial grown graphene on SiC. To characterize the epitaxial growth and correlate the structure with transport properties, the sheet resistance of graphene grown on SiC(0001) and SiC(000$\bar{1}$) have been studied via a 4-tip STM/SEM system. The SEM allows precise positioning of feedback controlled STM tips, enabling transport measurements on a nm-scale. While STM is used to characterize atomic size defect structures, step-bunches and nano-inhomogeneities can be identified in SEM. Sheet resistances were found to be independent from probe spacing indicating a 2d transport behavior but highly depending on ex-situ processing steps. Further in-situ annealing led to sheet resistances around $6 - 8$ k$\Omega/\square$. These values can be explained by diffusive transport theory [1] and correlate with the concentration of the nano-inhomogeneities. Structural defects induce a mobility gap as deduced from temperature-dependent transport measurements. The sheet resistance increased by a factor of three for elastically bend graphene layers across SiC step-bunches. [1] Adam *et al.*, PNAS, **104**, 18392 (2007)

O 57.4 Wed 16:45 H17

Electronic structure of epitaxial graphene on 3C-SiC(111)

— •Lydia Nemec, Volker Blum, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin

We present a study of the electronic structure of the carbon-rich surface phases on 3C-SiC(111), including quasi-freestanding graphene and intercalated phases. Our approach is based on density-functional theory (DFT) including van der Waals (vdW) dispersion terms in the Tkatchenko-Scheffler approach [1]. We use semilocal DFT (PBE+vdW functional) for our first-principles structure predictions. For the oxygen intercalated bilayer graphene, we consider an oxygen-rich interface passivating the Si dangling bonds [2]. Based on the predicted geometries, hybrid functionals (HSE06 and PBE0) are used to assess the electronic structure of: (1) the partially sigma-bonded "buffer layer" phase, (2) quasi-freestanding graphene up to three monolayers, and (3) hydrogen- and oxygen intercalated graphene phases. For the different phases, we discuss the changes of the electronic structure, addressing the influence of the intercalated material on the doping of the graphene and the charge transfer from the substrate to the graphene layer. We observe that in the intercalated phases graphene is decoupled from the substrate, making intercalation a promising approach for further studies.

[1] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).

[2] M.H. Oliveira *et al.*; Carbon **52**, 83-89 (2013).

O 57.5 Wed 17:00 H17

Graphene on cubic and hexagonal SiC: A comparative theoretical study

— Oleg Pankratov, •Stephan Hensel, Paul Götzfried, and Michel Bockstedte — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudstr. 7B2, D-91058 Erlangen

Epitaxial graphene grows on different SiC polytypes which possess distinct band gaps. We investigate the influence of polytypes on the graphene electronic spectrum employing density functional calculations with LDA and hybrid HSE functionals. We consider different buffer layer-graphene layer stackings as well as different substrate terminations.[1] We find a systematic displacement of the Dirac point relative to the valence-band edge as a function of the polytype hexagonality. The HSE values are in good agreement with available experimental results,[2,3] while LDA corroborates the trends. The Dirac point, the interface-related states, and the Fermi level follow similar polytype-dependent shifts, hence the graphene doping of the epilayer stays practically the same. For the AB stacked buffer and epilayer on Si-terminated SiC the Dirac spectrum exhibits an energy gap of 25-40 meV (depending on the polytype). On the contrary, for the AA stacking the Dirac cone remains intact. We suggest a symmetry-based analytical model which explains the origin of the gap and its absence for the AA geometry.

[1] Pankratov *et al.* Phys. Rev. B 86, 155432 (2012).

[2] Sonde *et al.*, Phys. Rev. B 80, 241406 (2009).

[3] Ristein *et al.*, Phys. Rev. Lett. 108, 246104 (2012).

O 57.6 Wed 17:15 H17

Phonons of graphene on SiC(0001)

— Stefan Fryska[1], Roland J. Koch[1], Felix Fromm[1], Alejandro Molina-Sánchez[2], •Ludger Wirtz[2], Martina Wanke[1,3], and Thomas Seyller[1,3] — [1]FAU Erlangen-Nürnberg — [2]University of Luxembourg — [3]TU Chemnitz

Epitaxial graphene (EG) on SiC(0001) can be grown on a wafer scale [1] but its charge carrier mobility is considerably lower than that of graphene flakes obstained by mechanical exfoliation. A previous study [2] of the temperature dependence of the mobility suggested that it is determined by remote phonon scattering with phonons of the buffer layer at the interface between EG and SiC(0001). The buffer layer, which is identical to the $(6\sqrt{3}\times6\sqrt{3})R30^\circ$ reconstruction of SiC(0001), consists of a monolayer of carbon atoms in a honeycomb structure. Due to a strong interaction with the substrate, the buffer layer has destorted π-bands and does not exhibit a Dirac cone [3]. In order to learn more about the phonons of the buffer layer we have carried out a study using high-resolution electron energy loss spectrscopy (HREELS) and Raman spectroscopy, accompanied by *ab-initio* calculations. We observe strong modifications of the phonons of the buffer layer with respect to weakly interacting, quasi-free standing graphene on SiC(0001). In particular, the Kohn anomaly is quenched, which agrees with the lack of a Dirac cone. [1] K. V. Emtsev et al., Nat. Mater. **8** (2009) 203. [2] F. Speck et al., Appl. Phys. Lett. **99** (2011) 122106. [3] K. V. Emtsev et al., Phys. Rev. B **77** (2008) 155303.

O 57.7 Wed 17:30 H17

Intercalation of hydrogen at the graphene/Ir(111) interface

— •Thorsten Balgar, Hyunil Kim, and Eckart Hasselbrink — Universität Duisburg-Essen, Universitätsstr. 5, D-45141 Essen

Epitaxially grown graphene on an iridium crystal exhibits a well known moire pattern due to the lattice mismatch of graphene and the Ir(111) surface. This leads to a buckling of the carbon layer and a lateral modulation of the chemical reactivity towards adsorbates [1,2]. Unlike intercalated metal atoms hydrogen cannot be directly detected with surface scientists' standard analysis tool box, namely XPS or AES. In our study we have used vibrational sum frequency generation (SFG) spectroscopy to monitor the stretching vibration of hydrogen chemisorbed on graphene [3]. The results are discussed in view of the intercalation of hydrogen and the local formation of graphane-like structures.

[1] C. Busse et al., Phys. Rev. Lett. 107 (2011) 036101 [2] J. Wintterlin et al., Surf. Sci. 603 (2009) 1841 [3] Kim et al., Chem. Phys. Lett. 546 (2012) 12

O 57.8 Wed 17:45 H17

Decoupling of Epitaxial Graphene on Ir(111) by Oxygen Intercalation

— •Søren Ulstrup[1], Rosanna Larciprete[2], Paolo Lacovig[3], Matteo Dalmiglio[3], Marco Bianchi[1], Jens Christian Johannsen[1], Federico Mazzola[1], Liv Hornekär[1], Fabrizio Orlando[4], Alessandro Baraldi[4], Silvano Lizzit[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Denmark — [2]CNR-Institute for Complex Systems, Roma, Italy — [3]Sincrotrone Trieste, Trieste, Italy — [4]Physics Department and Center of Excellence for Nanostructured Materials, University of Trieste, and IOM-CNR Laboratorio TASC, Area Science Park, Trieste, Italy

Epitaxial growth of graphene on transition metal surfaces is now a well-established method for obtaining extended layers of high quality graphene. However, interactions between graphene and its metal substrate are unwanted in applications typically requiring a mechanical transfer of the graphene. Here we demonstrate a different strategy based on decoupling the graphene from an Ir(111) substrate by oxygen intercalation. More specifically, we present evidence using photoelectron spectroscopy techniques that the intercalation results in an extended layer of hole-doped quasi free-standing graphene (QFG). Analysis of the electronic self-energy near the Fermi level reveals an extremely weak electron-phonon coupling in QFG. Finally, we find that abrupt deintercalation of oxygen occurs at elevated temperatures, which is accompanied by a modest etching of the graphene lattice.

O 57.9 Wed 18:00 H17

Transfer-free electrical insulation of epitaxial graphene from its metal substrate

— Silvano Lizzit[1], Rosanna Larciprete[2], Paolo Lacovig[1], Matteo Dalmiglio[1], Fabrizio Orlando[3,4], Alessandro Baraldi[3,4], Lauge Gammelgaard[5], •Lucas Barreto[6], Marco Bianchi[6], Edward Perkins[6], and

Philip Hofmann[6] — [1]Sincrotrone Trieste, Italy — [2]CNR-Institute for Complex Systems, Roma, Italy — [3]Physics Department and CENMAT, University of Trieste,Italy — [4]IOM-CNR Laboratorio TASC, Trieste, Italy — [5]Capres A/S, Lyngby, Denmark — [6]Institut for Fysik og Astronomi, Interdisciplinary Nanoscience Center (iNANO), Aarhus Universitet Denmark

High-quality, large-area epitaxial graphene can be grown on metal surfaces, but its transport properties cannot be exploited because the electrical conduction is dominated by the substrate. Here we show how to insulate epitaxial graphene from the Ru(0001) surface it is grown on by a step-wise intercalation of silicon and oxygen, and the eventual formation of a SiO_2 layer between the graphene and the metal. The reaction steps are followed by x-ray photoemission spectroscopy. The presence of a SiO_2 layer should insulate the metal from the substrate. In order to verify this, lateral transport measurements were performed using a nano-scale multipoint probe technique. The resistance obtained is substantially higher than expected for a clean ruthenium surface but consistent with that expected for graphene. Moreover, the data suggest two-dimensional electronic transport, as expected for graphene.

O 57.10 Wed 18:15 H17

Intercalation as a route to atomically sharp graphene/ferromagnet interfaces: Structural and electronic investigations — •Philipp Leicht, Konstantin Krausert, Lukas Zielke, and Mikhail Fonin — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The interface between graphene (G) and the substrate plays a vital role for the electronic properties of G. Apart from direct growth of G on a small number of substrates, a variety of metals can be intercalated between G and the substrate interface [1,2] and allow for the production of G on a large number of materials. In this work, we present the investigation of Ni intercalation underneath G on Ir(111). The atomic structure and electronic properties were investigated for samples with intercalated Ni ranging from a submonolayer to few monolayers.

For Ni intercalation underneath G/Ir(111), scanning tunneling microscopy shows strongly increased moiré corrugation as well as a decreased average distance of G/Ni/Ir(111) compared to G/Ir(111). The stronger corrugation is accompanied by considerable changes in the electronic structure of the G layer. The intercalation channels including the influence of defects and diffusion of intercalants within the graphene-metal interface are discussed for the two regimes of submonolayer and multilayer intercalation.

[1] M. Sicot et al. ACS Nano 6, 151 (2012) [2] L. Huang et al. Appl. Phys. Lett. 99, 163107 (2011)

O 57.11 Wed 18:30 H17

Magnetism of graphene/Ir(111) intercalation systems — •Régis Decker[1], Jens Brede[1], Nicolae Atodiresei[2], Vasile Caciuc[2], Stefan Blügel[2], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, D-30355 Hamburg — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungzentrum Jülich, D-52425 Jülich

The presence of intercalation compounds in graphite, i.e. impurities or layer(s) trapped between carbon sheets, can lead to changes in the transport, optical and catalytic properties compared to bulk graphite, or even to superconductivity. The intercalation of elements between graphene and its substrate can also influence the properties of graphene. Furthermore, this approach opens a new route to explore the behavior of graphene on a magnetic substrate.

Here, we present the local structure and magnetic properties of graphene on magnetic substrates, resolved by spin-polarized STM. The magnetic substrates are obtained by the intercalation of 3d elements (Co and Fe) between graphene and the Ir(111) surface [1]. In both cases, the atomic structure of the graphene layer is dominated by a highly corrugated Moiré pattern. Within the Moiré pattern different regions are identified. Interestingly, these regions show very different electronic and magnetic signatures in the experiments. The experimental observations are compared to state-of-the-art first principles density functional theory calculations.

[1] Atomic-scale magnetism of cobalt-intercalated graphene. R. Decker et al., accepted in Phys. Rev. B (Rapid Comm.).

O 57.12 Wed 18:45 H17

Deuteration kinetics of the graphene — •Alexei Nefedov[1], Alessio Paris[2], Nikolay Verbitskiy[3,11], Ying Wang[4], Alexander Fedorov[5,6], Danny Haberer[5], Martin Oetzelt[7], Luca Petaccia[8], Dmitry Usachov[6], Denis Vyalikh[6,9], Hermann Sagdev[10], Christof Woell[1], Martin Knupfer[5], Berndt Buechner[5], Lucia Calliari[2], Lada Yashina[3], Stephan Irle[4], and Alexander Grüneis[5,11] — [1]KIT, Leopoldshafen, Germany — [2]FBK-CMM, Trento, Italy — [3]MSU, Moscow, Russia — [4]Nagoya University, Nagoya, Japan — [5]IFW Dresden, Dresden, Germany — [6]St. Petersburg University, St. Petersburg, Russia — [7]BESSY II, Berlin, Germany — [8]Elettra, Trieste, Italy — [9]TU Dresden, Dresden, Germany — [10]MPI für Polymerforschung, Mainz, Germany — [11]University of Vienna, Vienna, Austria

The kinetics of the hydrogenation/deuteration reaction of graphene was studied by time-dependent x-ray photoemission spectroscopy (XPS). The graphene layer was then exposed to hydrogen or deuterium atomic gas beams, obtained by thermal cracking in a tungsten capillary at T=3000 K. After each step XPS of the C1s line was performed in order to measure H/C and D/C ratios. We have observed a strong kinetic isotope effect for the hydrogenation/deuteration reaction leading to substantially faster adsorption and higher maximum D/C ratios as compared to H/C (D/C~35% vs. H/C~25%).

O 57.13 Wed 19:00 H17

Intercalated thin films on Graphene/Ir(111) — •Hendrik Vita[1], Stefan Böttcher[1], Yuriy S Dedkov[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin — [2]SPECS Surface Nano Analysis GmbH, Voltastr. 5, D-13355 Berlin

The investigation of graphene/metal systems is interesting from fundamental as well as applications-oriented point of view. Here we report on the interaction of weakly and strongly bound intercalated metals (Cu vs. Ni) with graphene grown on Ir(111), using core and valence level photoemission spectroscopy. Studying the electronic structure of graphene in these interfaces reveals the effect of weak and strong interaction between graphene and the underlying intercalated thin film. The graphene/Ni/Ir(111) system shows a strong hybridization between the graphene π-band and the Ni 3d valence bands, which leads to the destruction of the graphene Dirac cone. The graphene/Cu/Ir(111) system, on the other hand, shows at first glance the properties of weakly bonded graphene (Dirac cone with a linear dispersion of the π-band) but with additional doping due to the donation of electrons by the intercalated Cu. Contrary to the weakly bonded scenario we observe a hybridization between the distinct Cu3d states and the graphene π-band.

O 58: Poster Session III (Solid-liquid interfaces; Scanning probe and other methods; Electronic structure theory; Spin-orbit interaction)

Time: Wednesday 18:15–21:45 Location: Poster B1

O 58.1 Wed 18:15 Poster B1

Temperature dependent wear experiments on the nanoscale — •Johannes Sondhauss[1], Harry Mönig[1], Harald Fuchs[1], and André Schirmeisen[2] — [1]Institute of Physics, University of Münster, Germany — [2]Institute of Applied Physics, University of Giessen, Germany

The importance of wear effects on small scales, e.g. with regard to moving mechanical components in MEMS, motivated increased efforts to analyze the basic mechanisms of wear at the nanoscale. Especially the atomic force microscope (AFM) has been proved useful to study wear effects on the atomic scale [1, 2]. Typically, the models used to describe the observed wear characteristics are based on Arrhenius kinetics and therefore a thermally activated characteristic is expected. However, a complete picture of the fundamental wear processes is still under debate. In this work we performed wear experiments as a function of temperature. We used Si-tips to wear single step edges on a KBr(001)-crystal. The measurements were conducted under UHV-conditions in a temperature range between 100 K and 300 K. We investigated the effect of different loads and, as a further important channel, we simultaneously measured the friction force acting between tip and sample during the wear process. With our results we are able to make an assessment if nanoscale wear can be described by an Arrhenius type model. In addition the influence of the different components of the acting normal and frictional stresses inside the contact area is discussed.

[1] Sheehan, Chem. Phys. Lett. 410, 151-155 (2005)

[2] Gotsmann and Lantz, Phys. Rev. Lett. 101, 125501 (2008)

O 58.2 Wed 18:15 Poster B1

Friction force microscopy on activated silicon surface — •Johanna Blass[1], Florian Hausen[1,2], Matthias Lessel[2], Peter Loskill[2], Marcel Albrecht[3], Nitya Nand Gosvami[1], Gerhard Wenz[3], Karin Jacobs[2], and Roland Bennewitz[1,2] — [1]INM - Leibniz-Institute for New Materials Campus D2 2, 66123 Saarbrücken, Germany — [2]Department of Experimental Physics, Saarland University, D-66041Saarbrücken, Germany — [3]Organic Macromolecular Chemistry Campus C4 2, Saarland University, D-66123 Saarbrücken, Germany

Surfaces with defined friction and adhesion properties are often required for technical applications such as strong mechanical links with high shearing but low peeling resistance. Therefore, we currently develop a novel surface material based on cyclodextrin assemblies with controlled anisotropy friction and adhesion characteristics. The interaction of two surfaces is based on host-guest interactions which are investigated by single molecule force spectroscopy and high resolution friction force microscopy. Immobilization results of cyclodextrin assemblies on activated silicon and gold are presented. Additionally, FFM experiments are presented which reveal an influence of the subsurface on an activated silicon surface. We found that friction forces on octadecyltrichlorosilane (OTS) self assembled monolayers as well as on siliconoxide decrease with a thicker oxide layer. The effect is attributed to a change in the van der Waals part of the effective interaction potential [1]. [1] P. Loskill, H. Hähl, T. Faidt, S. Grandthyll, F. Müller, and K. Jacobs, Adv. Coll. Interf. Sci. 107 (2012) 179182

O 58.3 Wed 18:15 Poster B1

Investigation of Tribological Properties of Mesoporous Alumina Membranes With Water Lubrication — •Florian Krämer[1], Felix Wählisch[2], Andreas Tschöpe[1], Rainer Birringer[1], and Roland Bennewitz[2] — [1]Universität des Saarlandes, Saarbrücken — [2]INM - Leibniz-Institut für Neue Materialien

Nanoporous membranes are interesting substrates for tribological applications because their porous structure allows to carry liquid lubricants into the friction interface directly.

In the present study, alumina templates with hexagonally arranged pores were synthezised by two step anodization of aluminum. The alumina-layer was separated by a voltage reversal technique. The barrier oxide at the pore-bottom was dissolved by chemical etching resulting in free-standing mesoporous membranes with complete open pore morphology (pore diameter about 60 nm). The membranes were mounted on a sample holder which allowed the direct contact with a water reservoir. Upon contact, the pores were filled with water by capillary forces to provide a thin water-layer on top of the membrane surface, where the tribological measurements were carried out.

The friction of a 500 μm ruby sphere on the membrane was characterized in the dry and the water-lubricated state by a reciprocal sliding tribometer. The wear track of the tribometer measurement was investigated by atomic force microscopy and scanning electron microscopy.

O 58.4 Wed 18:15 Poster B1

EC-STM study of the influence of gas adsorbates on the structure and morphology of Cu-monolayers on Au(1 1 1) and Pt(1 1 1) electrodes — •Christian Schlaup and Sebastian Horch — Center for Individual Nanoparticle Functionality (CINF), Department of Physics, Technical University of Denmark (DTU), DK–2800 Kongens Lyngby, Denmark

The electrodeposition of metals adlayers in general, and the underpotential deposition (upd) of metal (sub)monolayers in particular, is a major topic in interfacial electrochemistry and has been studied extensively. Often a strong dependence of the atomic structure of such metal upd layers on both, the substrate and the involved anionic species in the deposition electrolyte, was found.

In the present work, we studied the influence of neutral gas coadsorbates, such as dissolved CO_2 and CO, on the structure and morphology of Cu-upd layers on Au(1 1 1) and Pt(1 1 1) electrodes by means of cyclic voltammetry and EC-STM. Contrary to the case of purely anionic adsorbates, these gas adsorbates may not only influence the structure of the metal upd layer directly by coadsorption, but also indirectly due to attractive interactions with the underlying substrate. In order to be able to distinguish between these effects, we studied both, the Cu deposition in presence of gas adsorbates and the reaction of Cu-films on the introduction of gas adsorbates after their deposition from a *blank* electrolyte.

O 58.5 Wed 18:15 Poster B1

Two-dimensional metal-organic complexes as catalyst for the oxygen reduction reaction — •Benjamin Wurster[1], Doris Grumelli[1], Sebastian Stepanow[1], and Klaus Kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Two-dimensional metal-organic coordination networks (2D-MOCNs) consist of arrays of organic ligands coordinated with metal atoms self-assembled on metal surfaces. Due to the similarity with catalytically active sites in biological systems, the low-coordinated metal centers are considered to have promising properties in catalysis.

In this work, we will present the electrochemical characterization of 2D-MOCNs. The networks were prepared under ultra-high vacuum (UHV) conditions on Au(111). As organic ligands we used trimesic acid (TMA) and biphenyl-4,4'-dicarboxylic acid (BDA). The metal centers were single atoms of iron or manganese. The composition and structure of the networks were controlled and characterized by scanning tunneling microscopy in UHV. The sample is brought from UHV to the electrochemical cell through a transfer chamber in a controlled environment. Cyclic voltammetry experiments show that the networks catalyze the complete oxygen reduction towards H_2O and change the mechanism on Au(111) in alkaline media from a $2e^-$ pathway to a $4e^-$ $(2e^- + 2e^-)$ pathway.

O 58.6 Wed 18:15 Poster B1

Growth of imidazolium-based ionic liquid films on gold at low temperatures — Marcel Marschewski[1], Cornelia Kunz[1], •Oliver Höfft[2], Wolfgang Maus-Friedrichs[1], and Frank Endres[2] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Elektrochemie, TU Clausthal, Arnold-Sommerfeld-Str.6, 38678 Clausthal-Zellerfeld, Germany

Room temperature Ionic Liquids (RT-ILs) are a class of materials, which has recently gained enormous interest. Due to their exciting combination of properties they are of interest for numerous applications. Here we present our results for the growth of monolayers of imidazolium-based ionic liquid (ILs) films on gold at low temperatures. This was studied by electron spectroscopy using ultraviolet photoelectron spectroscopy (UPS, HeI) and metastable induced electron spectroscopy (MIES). We have prepared monolayers of 1-octyl-3-methyl-imidazolium bis(trifluoromethylsulfonyl)imide ([OMIm]Tf2N) on gold by vapour deposition at 140K. In contrast to the preparation of the monolayers at room temperature we observe an ordered growth of [OMIm]Tf2N beyond the first monolayer. Heating up to room temperature, results in the formation of a disordered film. In addition we present the interaction of cesium with thin films of imidazolium based ILs. Here we will focus on the solvation of cesium in these ionic liquid films. For the IL monolayers, grown on Si(100), we find a shift of the IL valence band states to higher binding energies during Cs adsorption.

O 58.7 Wed 18:15 Poster B1

Atomic resolution under ambient conditions with a qPlus force sensor — •Daniel S. Wastl, Alfred J. Weymouth, and Franz J. Giessibl — University of Regensburg, Regensburg, 93053, Germany

Frequency modulation atomic force microscopy (FM-AFM) is the preferred method to obtain high resolution AFM. So far, FM-AFM has mainly been employed in ultrahigh vacuum, but recently, atomic resolution has been obtained by FM-AFM in liquid [1] under ambient conditions with silicon cantilevers and by the qPlus sensor [2] in liquid [3]. The qPlus sensor is attractive, because it is self-sensing and thus does not require optical deflection measurements. Moreover, it has a higher quality factor in ambient conditions and should be competitive to silicon cantilevers in its noise performance [4, 5, 6]. However, we observed severe challenges due to a large change in cantilever damping on its transition from air to the adsorption layer / sample interface. Here, we provide atomic resolution on cleaved KBr (001) and of cleaved muscovite mica(001) under ambient conditions in a quality similar to data obtained in ultrahigh vacuum.

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[2] F. J. Giessibl, Appl. Phys. Lett., 76, 1470 (2000)
[3] T. Ichii et al, Jpn. J. Appl. Phys. 51 (2012)
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[5] E. Köstner, PhD thesis (2012)
[6] E. Wutscher at al, Rev. Sci. Instrum. 82, 093703 (2011)

O 58.8 Wed 18:15 Poster B1

Epitaxial order of self-assembled monolayers with attached molecular switches on Si(111), investigated by X-ray diffraction — •Christopher Weber[1], Michael Axman Petersen[2], and Stefan Kowarik[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin — [2]Institut für Chemie, Technische Universität Berlin, 10623 Berlin

Self-assembled monolayers (SAMs) can be used to chemically attach molecular switches to metal or semiconductor surfaces. The structure of the underlying linker SAM is often crucial for the switching efficiency of the system. In this case carboxyl-terminated alkyl-SAMs are used to couple molecular switches to a hexagonal Si(111) surface. The thickness, electron density and area per molecule of the SAM have been determined by X-ray reflectivity (XRR). The XRR results indicate that every second accessible Si-bond is occupied by an alkyl chain, in agreement with simulations. In addition to the out-of-plane information, the in-plane SAM structure and the epitaxial orientation of the SAM with respect to the Si(111) surface has been analyzed with grazing incidence X-ray diffraction (GIXD). We show that the alkyl-molecules form a highly stable SAM with a well-defined in-plane structure and epitaxial orientation relative to the Si(111) surface.

O 58.9 Wed 18:15 Poster B1

Work function change introduced by water on a halogen covered Pt(111) surface — •Florian Gossenberger and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

Anion adsorption on metal electrodes plays an important role in electrochemistry. Still, the knowledge about the microscopic structure of the interface between anion-covered electrodes and the electrolyte is still limited. We have used periodic density functional theory calculations to address the adsorption of halogen atoms (F, Cl, Br, I) on Pt(111). Typically, one expects that the adsorption of electronegative adsorbates will increase the work function. Interestingly enough, we find that the adsorption of halogens on a clean Pt(111) may lead to a significant decrease in the work function. According to our calculations, this behavior is due to a reduction in the surface dipole moment which itself depends on the charge distribution around the adsorbed halogen atoms.

Furthermore, we have studied the interaction of the adsorbed halogen atoms with single water molecules and whole water layers. We will in particular discuss the influence of the water molecules on the halogen-induced work function change of Pt(111).

O 58.10 Wed 18:15 Poster B1

Hierarchical self-assembly of polycyclic heteroaromatic stars into snowflake patterns: A route towards very large lattice constants — •Stefan-S. Jester, Eva Sigmund, Lisa M. Röck, and Sigurd Höger — Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Gerhard-Domagk-Strasse 1, 53121 Bonn, Germany

The self-assembly of rigid molecules with long alkyl/alkoxy side chains at the solution/solid interface allows an efficient approach towards 2D supramolecular crystalline surface patterns.[1,2] Scanning tunneling microscopy yields a submolecularly resolved insight into the adlayer structures and thus a conclusion on the driving forces for their formation. Of particular interest is how the nanoscale architectures depend on the design of the molecules, and how large unit cells can be derived. Here we present the two-dimensional self-assembly of polycyclic heteroaromatic star molecules with alkoxy side chains of distinct lengths on graphite. Depending on the chain length different dense and porous adsorbate patterns are observed. For $n = 12$ the frustrated self-assembly leads to hierarchically organized superstructures. Up to 10 molecules form triangular aggregates which pack densely into hexagonal patterns with very large (15.5 nm) lattice constants.[3]

[1] S.-S. Jester, N. Shabelina, S. M. Le Blanc, S. Höger, *Angew. Chem. Int. Ed.* **2010**, *49*, 6101. [2] S.-S. Jester, E. Sigmund, S. Höger, *J. Am. Chem. Soc.* **2011**, *133*, 11062. [3] S.-S. Jester, E. Sigmund, L. M. Röck, S. Höger, *Angew. Chem. Int. Ed.* **2012**, *51*, 8555.

O 58.11 Wed 18:15 Poster B1

Nanoscale surface patterning by molecular polygons: Can shape-persistent molecules behave like geometric tiles? — •Stefan-S. Jester, Nina Schönfelder, Eva Sigmund, and Sigurd Höger — Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Shape-persistent macrocycles are formed by cyclooligomerization of respective acetylene-terminated half-ring structures under oxidative coupling conditions and subsequent separation of the crude product by recycling gel permeation chromatography. Self-assembled monolayers of the resulting monodisperse compounds are investigated by scanning tunneling microscopy at the interface of 1,2,4-trichlorobenzene and highly oriented pyrolytic graphite. The macrocycles ($3 \leq n \leq 6$) can be viewed as equilateral molecular polygons (triangles, squares, pentagons, hexagons) that consist of rigid backbones and long flexible alkoxy side chains. We particularly focus on dithiophene corner units linked by p-phenylene-ethynylene-butadiynylene rods. The length of the latter can be systematically increased, and the related polygon sizes define the pattern periodicities. Cocrystallization - for example after mixing triangles and hexagons - increases the complexity of the resulting patterns. One fundamental question is how and to which extent the concepts of discrete geometry can be transferred to design patterns with unit cells far beyond 20 nm. [1] S.-S. Jester, E. Sigmund, S. Höger, *J. Am. Chem. Soc.* **2011**, *133*, 11062.

O 58.12 Wed 18:15 Poster B1

Self-assembled monolayers of molecular spoked wheels: Scanning tunneling microscopy — •Stefan-S. Jester[1], Vikas Aggarwal[1], Alissa Idelson[1], Alexander Thiessen[2], Daniel Kalle[1], Dominik Würsch[3], Thomas Stangl[3], Florian Steiner[3], Jan Vogelsang[2], John M. Lupton[2,3], and Sigurd Höger[1] — [1]Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany — [2]Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA — [3]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

Shape-persistent molecular polygons can be viewed as a combination of rigid molecular rod units and corners. The stiffness of the molecules is related to the persistence length of the sides, arylene-alkynylene rods, and the rotational degree of freedom of the corner units. For corner/side numbers $n < 3$ such molecules can deform out of their plane by rotation of the corner joints. Nevertheless, shape-persistence can be established by intraannular rigid spoke units to yield molecular spoked wheels.[1,2] STM investigation of adlayers of these molecules and its smaller subunits at the solid/liquid interface (e.g. 1-octanoic acid/graphite) yields a submolecularly resolved insight into the molecular architectures and their adsorbate pattern formation.

[1] D. Mössinger, D. Chaudhuri, T. Kudernac, S. Lei, S. De Feyter, J. M. Lupton, S. Höger, *J. Am. Chem. Soc.* **2010**, *132*, 1410. [2] D. Mössinger, J. Hornung, S. Lei, S. De Feyter, S. Höger, *Angew. Chem. Int. Ed.* **2007**, *46*, 6802.

O 58.13 Wed 18:15 Poster B1

Two-photon photoemission of thin CoO-Films on Ir(100)-(1x1) — •Sebastian Otto and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Two-photon photoelectron spectroscopy is used to study unoccupied states on thin CoO films grown epitaxially on Ir(100)-(1x1). Unoccupied states were found on various reconstructions of one Co-monolayer thick films with different oxygen amounts [1] and CoO(111) films [2] with thickness of up to ten bilayers. Ultrathin CoO films with a Co amount of about one monolayer show an increasing energy of the unoccupied state from 2.36 to 4.03 eV and an increase of the work function from 5.18 to 6.12 eV with increasing oxide content. For low coverages the observed states are in good agreement with scanning tunneling spectroscopy measurements [3]. On thicker CoO(111) films an increase of the energy from 3.36 to 3.62 eV with film thickness is found, while the work function decreases from 6.01 to 5.69 eV. A comparison with calculations for bulk CoO [4] suggests that the observed states correspond to unoccupied Co 3d orbitals.

[1] M. Gubo, C. Ebensperger, W. Meyer, L. Hammer and K. Heinz. Phys. Rev. B 83 (2011) 075435.
[2] K. Biedermann, M. Gubo, L. Hammer and K. Heinz. J. Phys.:

Condens. Matter 21 (2009) 185003.
[3] C. Tröppner. Dissertation, Universität Erlangen-Nürnberg (2011).
[4] V. I. Anisimov, F. Aryasetiawan and A. I. Lichtenstein. J. Phys.: Condens. Matter 9 (1997) 767.

O 58.14 Wed 18:15 Poster B1

Photon energy and polarization dependent photoemission from Ag(001) using a laboratory light source with time-of-flight setup — •Michael Huth[1], Cheng-Tien Chiang[1,2], Jürgen Kirschner[1], and Wolf Widdra[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

We use a high-harmonic generation light source for time-of-flight angle-resolved photoemission spectroscopy at 4 MHz on Ag(001). With 17 eV and 20 eV photon energy we observed dispersive features of the bulk electronic structure starting from 7 eV below the Fermi level. The dispersion depends on the chosen linear polarization of the incident light due to symmetry selection rules. Our results demonstrate efficient application of momentum-resolved high-repetition rate time-of-flight spectroscopy [1].

[1] C.-T. Chiang, A. Blättermann, M. Huth, J. Kirschner, and W. Widdra, Appl. Phys. Lett. **101**, 071116 (2012)

O 58.15 Wed 18:15 Poster B1

Reduced Ceria Surfaces: Ab initio computation of the electronic structure with the GGA+U method — •Alexander Hampel, Daniel Grieger, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg, Germany

This work deals with the investigation of the atomic and electronic structure of oxygen reduced ceria (111) surfaces within the *GGA+U* formalism as implemented in the Vienna ab initio Simulation Package (VASP). Within the *GGA+U* formalism one can take account of the strongly correlated *f*-states. The ab initio investigation starts with the determination of the correct lattice constant and the choice of the Hubbard-U value in the bulk to reproduce a correct insulating band gap. Using periodic supercells the electronic structure of the surface is calculated and the main properties of the clean surface are pointed out. This leads to the investigation of the oxygen vacancies. The change of the ceria structure by the lack of an oxygen atom on the surface and in the sub-surface are investigated. Surface energies give a good estimation of the probability for the (111) surface to appear and formation energies estimate the stability of the defects. Finally, we have a look on the change of electronic structure initiated by the vacancies, mainly the density of states. So one can see the advantages of the *GGA+U* treatment of the *f*-states and where the strongly correlated electrons are located.

O 58.16 Wed 18:15 Poster B1

Scanning tunneling spectroscopy of the highly correlated electron system Sn on Si(111) — •Jochen Settelein[1], Philipp Höpfner[1], Jörg Schäfer[1], Gang Li[2], Werner Hanke[2], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg — [2]Inst. für Theoret. Physik und Astronomie, Universität Würzburg

Two-dimensional electron systems can be realized at the surface of semiconductors by metal atom adsorption. A particularly intriguing scenario emerges for submonolayer coverages, since strong electron correlations come into play. At the same time, if a triangular lattice symmetry is chosen, any concomitant spin order faces the problem of geometric frustration. Here we address these intriguing questions by studying the reconstruction of Sn on Si(111) which, contrary to naive expectation of a metallic state, is suggestive of a Mott-Hubbard insulator at low temperatures [1].

We have studied the electronic properties by scanning tunneling microscopy and spectroscopy (STS). The tunneling spectra at low temperature show a characteristic dip around the Fermi level, indicative of insulating behavior. The spectral features on either side can well be interpreted in terms of lower and upper Hubbard band, respectively. Above 40 K the differential conductivity at the Fermi level increases gradually. The results are consistent with advanced many-body modeling by a dynamical cluster approximation. The STS results support the view as Mott insulator without a sharp transition as a function of temperature, and point at the role of longer-ranged correlations.

[1] S. Modesti *et al.*, Phys. Rev. Lett. **98**, 126401 (2007).

O 58.17 Wed 18:15 Poster B1

Scanning tunneling microscopy and spectroscopy of the phase change alloy $Ge_2Sb_2Te_5$ — •Jens Kellner[1], Christian Pauly[1], Marcus Liebmann[1], Alessandro Giussani[2], Raffaella Calarco[2], and Markus Morgenstern[1] — [1]II. Phys. Inst. B, RWTH Aachen University and JARA-FIT, Germany — [2]Paul Drude Institut für Festkörperelektronik, Berlin, Germany

We use scanning tunneling microscopy (STM) in ultrahigh vacuum (UHV) to probe the local atomic structure and the electronic properties of the phase change alloy $Ge_2Sb_2Te_5$(0001) grown on Si(111) by molecular beam epitaxy. In order to obtain a clean surface, the mixed native oxides on the GST surface were removed by dipping the sample in de-ionized water followed by annealing at 200°C in UHV [1]. We realized images with atomic resolution in constant-current mode at different voltages in order to distinguish different chemical elements on the surface. Local variations in the atomic corrugation and lattice constants are found and analyzed in detail. Using the spectroscopy mode, we find a band gap of about 500 meV. A p-type doping becomes apparent in agreement with photoelectron spectroscopy data.

[1] Z. Zhang et al., Appl. Surf. Sci. 256, 7696 (2010).

O 58.18 Wed 18:15 Poster B1

Characterization of single crystalline phase change materials by angular-resolved photoemission spectroscopy: Evidence for topological band inversion — •Christian Pauly[1], Marcus Liebmann[1], Alessandro Giussani[2], Jens Kellner[1], Sven Just[1], Jaime Sánchez-Barriga[3], Andrei Varykhalov[3], Oliver Rader[3], Raffaella Calarco[2], and Markus Morgenstern[1] — [1]II. Phys. Institut B, RWTH Aachen University and Jara Fit, Germany — [2]Paul Drude Institut für Festkörpelektronik, Berlin, Germany — [3]Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany

Phase change materials based on Ge-Sb-Te ternary alloys have been widely used as optical rewritable data storage media. They are also regarded as a promising candidate for a nonvolatile storage system (PCRAM), which exploits the high electrical contrast between the amorphous and the crystalline phase. Using angular-resolved photoemission spectroscopy (ARPES) we probe the band structure of epitaxially grown single crystalline phase change materials, $Ge_2Sb_2Te_5$ and GeTe. The samples are either transferred in-situ using a home-made UHV shuttle or cleaned by dipping in de-ionized water for 1min and annealing to 250°C in UHV [1]. ARPES maps show well defined bands for both materials. Interestingly, the band structure of $Ge_2Sb_2Te_5$ reveals a prominent bulk valence band which crosses E_F, forming two maxima around the $\bar{\Gamma}$-point. According to recent DFT calculations [2], this is a hint for a spin-orbit induced band inversion which is a requirement for topological properties. [1] Z. Zhang et al., Appl. Surf. Sci. 256, 7696 (2010) [2] J. Kim et al., Phys. Rev. B 82, 201312 (2010)

O 58.19 Wed 18:15 Poster B1

Van der Waals adsorption of Xe on Cu(100) — •Anuschka Schaffner, Alexander Potzuweit, Hagen Allmrodt, Lars Kraft, and Heinz J. Jänsch — AG Oberflächen, Fachbereich Physik, Philipps-Universität Marburg, Deutschland

We employ Nuclear Magnetic Resonance (NMR) of ^{129}Xe to investigate the adsorption of Xenon on metal single crystal surfaces, here Cu(100). On various metals Xe shows a reasonably strong shift in the work function and in the TPD desorption temperature. Calculations show the mixing of the Fermi-level electrons with the wavefunctions of Xenon. This local density of states (LDOS) manifests itself in the NMR chemical shift (Knight shift) and/or T_1 relaxation (Korringa relaxation). The such visible hyperfine interaction is a pure ground state property and is thus accessible to theoretical treatment in a LDOS determination in DFT or other appropriate calculation.

Experimentally Xe is adsorbed in a constant flux of atoms impinging on the surface, typically 4 ML/s or 40 ML/s. By controlling the crystal's temperature the formation of either a bulk or an equilibrium of ad- and desorbing atoms can be established. To achieve the necessary sensitivity, spin exchange optical pumping of Rubidium/Xenon mixtures is employed, resulting in a signal gain of 5 orders of magnitude.

In first experiments the chemical shift σ of ^{129}Xe on Cu(100) is determined and will be contrasted to the shift on Cu(111). The shift of Xe/Cu(100) is substantially smaller as compared with Xe/Cu(111). This is attributed to the narrow surface state at the Fermi level of Cu(111) which is missing at the Cu(100) surface.

O 58.20 Wed 18:15 Poster B1

Dielectric Properties of Functional Oxide thin-films from First Principles — •Jawad Alsaei[1], Neal Alford[2], Paul Tangney[1], and Arash A. Mostofi[1] — [1]Departments of Materials and Physics, Imperial College London, SW7 2AZ, United Kingdom. — [2]Department of Materials, Imperial College London, SW7 2AZ, United Kingdom.

Perovskite oxide materials show a wide range of physical properties that make them interesting both technologically and scientifically. Particular attention has been drawn to perovskites in thin-film form in order to meet the demand of manufacturing smaller industrial components such as advanced integrated electronic devices.

The optical properties of thin-film perovskite oxides can differ significantly from those of the bulk due to several factors, such as the mismatch strain imposed by the substrate, cation substitution, point defects, etc. We investigate, from first principles, the effect of some of these factors on the optical properties of functional oxide materials ($BaTiO_3$ and $SrTiO_3$).

First, it is found that the refractive index, at (400-1600 nm), increases with applied uni-axial strain. Second, the optical properties of $Ba_xSr_{1-x}TiO_3$ (BSTO) solid solutions are studied using both the supercell and the virtual-crystal approximation (VCA) approaches. It is found, surprisingly perhaps, that the two methods agree remarkably well. Third, the effect of Sr content in BSTO is investigated. It is found that the refractive index decreases almost linearly as the Sr:Ba ratio increases. Finally, the effect of Oxygen vacancies is studied.

O 58.21 Wed 18:15 Poster B1

Tb on Bi thin films - Conductivity and surface diffusion — ●P. Kröger[1], D. Lükermann[1], S. Sologub[2], H. Pfnür[1], M. Horn von-Hoegen[3], C. Klein[3], and C. Tegenkamp[1] — [1]Inst. f. Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover — [2]Nat. Acad. of Science, Nauky Av. 46, 03028 Kyiv, Ukraine — [3]Dep. of Physics and CeNIDE, Uni Duisburg-Essen, Lotharstraße 1, 47057 Duisburg

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as a low carrier concentration and a large mobility. Furthermore, the surface states reveal a pronounced Rashba splitting and the conductivity can be well discriminated from bulk contributions if thin films are grown epitaxially on Si(111) substrates, making surface related effects accessible even in macroscopic conductance measurements. In this conclusion the adsorption of various adsorbates on Bi(111) will be discussed. Adsorption of magnetic atoms (Fe, Co and Tb) at low T is accompanied by a transition from Weak Anti- to Weak Localization in magneto-transport measurements, related to the break of time reversal symmetry. Furthermore there a significant increase of carrier concentration due to hybridization effects has been found. **[1]** For Tb, additionally, surface diffusion of Tb-atoms even at T≈10 K needs to be considered. Visible as a low coverage minimum in conductance during adsorption. A simple nucleation theory approach describes the data very well. Tb turns out to be an even stronger scatterer than the other magnetic atoms like Co or Fe. **[1] Lükermann et. al, PRB 84 (2012), accepted.**

O 58.22 Wed 18:15 Poster B1

Barrier free sub-surface incorporation of magnetic impurities into the Bi(111) surface: Manipulation of the protected surface state — ●C. Klein[1], P. Zahl[2], N. Vollmers[3], U. Gerstmann[3], D. Lückermann[4], D.P. Acharya[2], P. Sutter[2], H. Pfnürr[4], C. Tegenkamp[4], W.-G. Schmidt[3], and M. Horn-von Hoegen[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]CFN, Brookhaven National Laboratory, Upton, New York 11973, USA — [3]Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — [4]Institut for Solid State Physics, University of Hannover, Appelstr. 2, 30167 Hannover, Germany

Due to the large spin orbit coupling electron backscattering in the Bi(111) surface state is strongly suppressed: the surface state is protected. In order to identify possible scattering mechanism we performed low temperature scanning tunneling microscopy (LT-STM) measurements in which sub-monolayer amounts of Fe and Co were deposited into the STM at 5K. After deposition the metal atoms are immediately embedded in a sub-surface site, as they are not present in topology. In dI/dV images the embedded impurities, however, become apparent as they are surrounded by a pronounced anisotropic threefold electronic scattering pattern with lateral dimensions of more than 10 nm. Calculations indeed confirm a barrier free incorporation of the impurities into the first Bi-Bilayer even at such low temperatures. Large changes of the scattering pattern as function of the tunneling bias reflects the dispersion of the occupied and unoccupied surface state of Bi(111).

O 58.23 Wed 18:15 Poster B1

Barrier free sub-surface incorporation of magnetic impurities into the Bi(111) surface: Manipulation of the protected surface state — ●C. Klein[1], P. Zahl[2], N. Vollmers[3], U. Gerstmann[3], D. Lückermann[4], D.P. Acharya[2], P. Sutter[2], H. Pfnür[4], C. Tegenkamp[4], W.G. Schmidt[3], and M. Horn-von Hoegen[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]CFN, Brookhaven National Laboratory, Upton, New York 11973, USA — [3]Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — [4]Institut for Solid State Physics, University of Hannover, Appelstr. 2, 30167 Hannover, Germany

Due to the large spin orbit coupling electron backscattering in the Bi(111) surface state is strongly suppressed: the surface state is protected. In order to identify and tune possible scattering mechanisms we performed low temperature STM (LT-STM) measurements in which sub-monolayer amounts of Fe and Co were deposited into the STM at 5K. After deposition the metal atoms are immediately embedded into a sub-surface site, as they are not present in topology. In dI/dV images the embedded impurities, however, become apparent as they are surrounded by a pronounced anisotropic threefold electronic scattering pattern with lateral dimensions of more than 10 nm. DFT calculations indeed confirm a barrier free incorporation of the impurities into the first Bi-Bilayer even at such low temperatures. Large changes of the scattering pattern as function of the tunneling bias reflects the dispersion of the occupied and unoccupied surface states of Bi(111).

O 58.24 Wed 18:15 Poster B1

Band bending in the unoccupied electronic structure of Bi_2Se_3 — ●Ch. Langenkämper[1], A. Zumbülte[1], A. B. Schmidt[1], M. Donath[1], T. Förster[2], P. Krüger[2], M. Bianchi[3], R. C. Hatch[3], P. Hofmann[3], J. Mi[4], B. B. Iversen[4], G. Mussler[5], and D. Grützmacher[5] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Institut für Festkörpertheorie, Universität Münster, Germany — [3]Department of Physics and Astronomy, Aarhus University, Denmark — [4]Department of Chemistry, Aarhus University, Denmark — [5]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

We report on angle- and spin-resolved inverse photoemission measurements on the topological insulator Bi_2Se_3.

Vacancies and adsorbates on surfaces of topological insulators are known to modify the charge density at the surface. The resulting band bending leads to an energetic shift of the bandstructure and the evolution of Rashba-split surface states. With regard to possible future applications and the interpretation of surface reactions, the influence of this band bending on the unoccupied electronic structure plays an important role. Here, we examine the time evolution of the band structure for two different sample systems: an MBE-grown thin film and a bulk crystal. Especially the evolution of new structures due to surface reactions will be discussed on the basis of theoretical calculations. Additionally, we investigate the influence of the threefold crystal symmetry, which causes differences between the surface states in $\overline{\Gamma}\,\overline{M}$- and $\overline{\Gamma}\,\overline{M}'$-direction.

O 58.25 Wed 18:15 Poster B1

Imaging the local transport field of a Bi2Se3 surface — ●Sebastian Bauer, Alexander M. Bernhart, Mark R. Kaspers, Rolf Möller, and Christian A. Bobisch — Faculty of Physics, Center of Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Since the prediction of the unique properties of topological insulators in 2007 [1] those new material class has become one of the most studied materials in condensed matter physics. To study the lateral variation of the electrochemical potential we performed scanning tunneling potentiometry (STP) [2] on the surface of thin films of Bi2Se3 grown on a Si(111) substrate. The films were prepared according to Zhang et al. [3]. All experiments, the preparation as well as the analysis, were carried out in situ under UHV conditions. For the STP measurements two tips of a four probe scanning tunneling microscope (STM) are contacted to the surface to apply an electric field parallel to the surface. A third tip simultaneously maps the topography and the local electrochemical potential of the surface [4]. We present first STP results showing a spatial variation of the electrochemical potential of the Bi2Se3 surface. In addition, to the transport field the thermovoltage of the tunneling barrier is detected. The two signals can be disentangled by reversal of the lateral current, because that changes the sign of the transport field leaving the thermovoltage unchanged. [1] L. Fu, C.

Kane, and J. Mele, Phys. Rev. Lett. 98, 106803 (2007)[2] P. Muralt, D. Pohl, Appl. Phys. Lett. 48, 514 (1986)[3] G. Zhang, et al., Appl. Phys. Lett. 95, 053114 (2009)[4] J. Homoth, et al., Nano Letters 9, 1588 (2009)

O 58.26 Wed 18:15 Poster B1

Unoccupied Surface States of Si(111)($\sqrt{3}\times\sqrt{3}$)R30°-Bi — •F. Rühl[1], D. Niesner[1], Th. Fauster[1], P. Sessi[2], M. Bode[2], M. Trioni[3], S. Achilli[3], G. Bihlmayer[4], and E. V. Chulkov[5] — [1]Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [3]Dipartimento di Scienza dei Materiali and CNISM, Universitá degli Studi di Milano-Bicocca, Via Cozzi 53, 20125 Milano, Italy — [4]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — [5]Donostia International Physics Center, 20018 San Sebastián, Basque Country, Spain

The ($\sqrt{3}\times\sqrt{3}$)R30°-reconstructed trimer phase Bi on Si(111) shows giant Rashba spin-splitting in UV photoemission [1]. In the present study, the unoccupied states were investigated by monochromatic ($h\nu$= 3.1, 4.65 eV) and bichromatic ($h\nu$= 1.55+4.65 eV) two-photon-photoemission. From the photon energy and polarization dependence, surface states are identified and a downward dispersing band 3.28 eV above the Fermi level was found. In addition, surface states exist at 2.58 eV and 2.23 eV at the $\overline{\Gamma}$-point and at the $\overline{\mathrm{M}}$-Point at 2.5 eV. The workfunction is 4.64 eV. The photovoltage for flatband conditions was determined to 70 meV. The Fermi level is located 0.22 eV above the valence band maximum. A long-lived feature with a lifetime >15 ps was identified at 0.73 eV. The results are compared with scanning tunneling spectroscopy data and density functional theory calculations.

[1] K. Sakomoto *et al.*, Phys. Rev. Lett. **103**, 156801 (2009)

O 58.27 Wed 18:15 Poster B1

Adsorption of organic layers on the giant spin orbit split BiAg$_2$ surface alloy — •Maren C. Cottin[1], Johannes Schaffert[1], Jorge Lobo-Checa[2], J. Enrique Ortega[2,3,4], Andrew L. Walter[4], Christian A. Bobisch[1], and Rolf Möller[1] — [1]Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Centro de Física de Materiales CSIC/UPV-EHU-Materials Physics Center, Manuel Lardizábal 5, E-20018 San Sebastián, Spain — [3]Departamento Física Aplicada I, Universidad del País Vasco, E-20018 Donostia-San Sebastián, Spain — [4]Donostia International Physics Center, Manuel Lardizábal 4, E-20018 San Sebastián, Spain

The emerging field of spintronic devices has recently triggered a lot of research effort on materials exhibiting a spin-splitting of their electronic states. Recently, surface alloys such as PbAg$_2$, BiCu$_2$ or BiAg$_2$ have gathered a lot of attention due to the giant spin orbit splitting of their surface states. At the same time organic molecules have already become important electronic building blocks of modern electronic devices.

To study the effect of the adsorption of organic layers on such giant spin split surface states, scanning tunneling microscopy (STM) experiments have been performed, e.g. on the archetype organic molecule 3,4,9,10 - perylene tetracarboxylic dianhydride acid (PTCDA) adsorbed on BiAg$_2$. The STM images show ordered layers exhibiting different molecular superstructures.

O 58.28 Wed 18:15 Poster B1

Unoccupied surface states of p-type topological insulators — •Volker Hermann[1], Daniel Niesner[1], Thomas Fauster[1], Eugene V. Chulkov[2], Ziya S. Aliev[3], Mammadb B. Babanly[3], and Imamaddin R. Amiraslanov[4] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Donostia International PhysicsCenter (DIPC), 20018 San Sebastián/Donostia, Basque Country, Spain — [3]General and Inorganic Chemistry Department, Baku State University, Baku, AZ1148, Azerbaijan — [4]Institute of Physics, Azerbaijan National Academy of Science, Baku, AZ1143, Azerbaijan

Density functional theory calculations predict a topological surface state (TSS) for SnSb$_2$Te$_4$ [1]. No Dirac point was found in UV photoemission. The material therefore is doped p-type.

Two-photon photoemission was used to investigate the unoccupied band structure. The Dirac point is found 0.3 eV above the Fermi level with a group velocity of 3.4 eVÅ. A work function of about 5.25 eV was measured. Time-resolved experiments show that the TSS is not only populated optically by the pump pulse but also indirectly by refilling from the bulk conduction band similar to the case of Bi$_2$Se$_3$ [2]. From a rate-equation model a lifetime of about 45 fs was found. A small lifetime is explained by scattering to the partly depleted bulk valence band.

[1] T.V. Menshchikova *et al*, Appl. Surf. Sci., in press
[2] J.A. Sobota *et al.*, Phys. Rev. Lett. **108**, 117403 (2012)

O 58.29 Wed 18:15 Poster B1

Relaxation dynamics in laser-excited metals under non-equilibrium conditions — •Benedikt Y. Mueller and Bärbel Rethfeld — Technical University Kaiserslautern, Germany

When an ultrashort laser pulse irradiates a metal, energy is absorbed by the electron system which is driven out of thermal equilibrium on a femtosecond timescale. Due to electron-electron collisions a new thermodynamical equilibrium state within the electron system is established in a characteristic time, the so-called thermalization time. The absorbed energy of the electrons will be further transferred to the phononic system. The thermalization time as well as the electron-phonon coupling strength [1] both strongly depend on the material properties and the excitation type. Furthermore, a non-thermalized electron gas couples differently to the phononic system as a thermalized one [2]. In order to follow the relevant microscopic dynamics without the need to assume thermalized electrons, we apply complete Boltzmann collision integrals to describe the transient electron distribution due to excitation, thermalization and relaxation. We implement the density of states of real materials in our approach [3]. As a result of our simulations, we extract the electron thermalization time and the electron-phonon coupling under non-equilibrium conditions. Examples are given for aluminum, gold an nickel.

[1] Z. Lin et al., Phys. Rev. B 77, 075133 (2008)
[2] B. Rethfeld et al., Phys. Rev. B 65, 214303 (2002)
[3] B. Y. Mueller et al., AIP Conf. Proc. 1461, 609 (2012)

O 58.30 Wed 18:15 Poster B1

Dynamical Simulation of Photoinduced Electron Transfer in Nitrile-Substituted Alkanethiolate Self-Assembled Monolayers Adsorbed at the Au(111) Surface — •Veronika Prucker[1], Pedro B. Coto[2], Óscar Rubio-Pons[1], Michel Bockstedte[1], Haobin Wang[3], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Departamento de Química-Física, Universidad de Alcalá, Alcalá de Henares, Madrid, Spain — [3]Department of Chemistry and Biochemistry, MSC 3C, New Mexico State University, Las Cruces, New Mexico 88003, USA

Photoinduced electron transfer dynamics in self-assembled monolayers consisting of nitrile substituted short-chain alkanethiolate molecules adsorbed at the Au(111) surface is studied. The method employed is based on a model Hamiltonian, which is determined by first-principles electronic structure calculations [1], and dynamical simulations. In comparison with experimental results [2], we analyze the influence of the orbital-symmetry of the donor state and the length of the aliphatic spacer chain of the monolayer on the electron transfer process. Moreover, the mechanisms controlling the electron transfer times are discussed.

[1] I. Kondov *et al.*, J. Phys. Chem. C 111, 11970 (2007).
[2] F. Blobner *et al.*, J. Phys. Chem. Lett. 3, 436 (2012).

O 58.31 Wed 18:15 Poster B1

Electronic lifetimes in a 2D electron gas in Bi/Cu(111): Screening effects and consequences for the spin structure — •Svenja Vollmar, Andreas Ruffing, Sebastian Jakobs, Alexander Baral, Steffen Kaltenborn, Mirko Cinchetti, Stefan Mathias, Martin Aeschlimann, and Hans Christian Schneider — University of Kaiserslautern

We compare energy resolved lifetimes in the quantum-well system Bi/Cu(111) as obtained from time- and angle-resolved 2-photon photoemission spectroscopy with the results of a Rashba model for the quantum-well bands with parameters extracted from the experiment.

Since the bulk screening constants for Bi and Cu are very different, we derive the correct statically screened potential for the Coulomb interaction of the electrons in the Bi-layer on the Cu-substrate.

We find that the measured lifetimes plateau around the intersection point cannot even qualitatively be explained on the basis of the Rashba model. Only by the ad-hoc introduction of a more complicated spin structure by assuming a k-dependent spin mixing, the calculated lifetimes qualitatively agree with experiment. Our results indicate that the spin-orbit coupling leads to band-structure effects beyond those described in a pure Rashba model.

O 58.32 Wed 18:15 Poster B1

Temporal Evolution of Excited Electrons in the Ni(111) Image-Potential States — •Beatrice Andres[1], Paul Weiss[1], Marko Wietstruk[1], Anke B. Schmidt[2], Markus Donath[2], and Martin Weinelt[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — [2]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

In ferromagnetic materials electronic relaxation times differ for electrons with majority and minority spin. Besides spin-conserving decay, which mainly occurs through inelastic electron-electron scattering, relaxation is also caused by spin-flip processes. Additionally the interaction of electrons with phonons and defects give rise to spin-dependent dephasing rates.

In spin- and time-resolved two-photon-photoemission experiments (2PPE) we populate the $n = 1$ and $n = 2$ image-potential states on Ni(111) with the third harmonic ($3h\nu \approx 5.0$ eV) of our Ti:Sa laser. We can excite electrons from different initial states by changing the photon energy and thus modify the spin polarization created in the image states. Probing the electronic structure after a variable time delay with the fundamental ($1h\nu \approx 1.67$ eV) enables us to study spin-dependent differences in image-state lifetimes and temporal evolution of linewidths. Our results indicate diversities in the decay channels and dephasing processes for majority- and minority-spin electrons.

O 58.33 Wed 18:15 Poster B1

Combined XPS and XAS Analysis Using the Software UNIFIT 2013 — •Ronald Hesse, Reinhard Denecke, and Martin Welke — Universität Leipzig, Wilhelm-Ostwald-Institut, 04103 Leipzig, Linnéstr. 2

A combination of X-ray absorption spectroscopy (XAS) and x-ray photoelectron spectroscopy (XPS) using synchrotron radiation with variable energy and polarized soft x-rays with high resolution and high flux is a powerful technique to observe atomic compositions and electronic state of surfaces of materials. In order to extract the maximum of information of the studied material a spectrum fit for both methods has to be done. The newest version of the software UNIFIT allows the combined spectrum processing and peak fit of XPS and XAS measurement data. The different theoretical description of the spectral background of XA spectra was implemented in the software. Additionally, the input routine was expanded for the reading of four special XAS data formats (NEXAFS, BESSY-EMP/2, LUND-MAXlab Scan Zeiss, 1. Column: Photon Energy - 2. Column: Intensity). The peak fit of a XA and XP spectrum of Ti 2p as well as a XMCD study of a thin Co film on BaTiO2 demonstrate the new possibilities of the improved software UNIFIT 2013.

O 58.34 Wed 18:15 Poster B1

Numeric atom-centered basis set with valence correlation consistency from H to Ar — •Igor Ying Zhang, Xinguo Ren, Patrick Rinke, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

Numeric atom-centered orbitals are appealing for electronic structure theory, particularly density-functional theory (DFT), because the occupied effective single-electron orbitals required to construct the density can be represented by rather efficient, compact, yet transferable NAO basis sets [1]. It is well known, however, that for perturbative approaches beyond DFT (RPA, MP2, GW, etc.) the basis set convergence is much slower. We here present a prescription for numeric atom-centered correlation consistent basis sets, coined NAO-VCC-XZ (X=D,T,Q,5). Like their Gaussian based counterparts [2], these NAO-VCC-XZ basis sets provide a much more systematic convergence to the complete basis set limit, reducing the basis set superposition error and giving rise to extrapolation techniques for total energies,binding energies, etc. The advantage of NAOs over Gaussians is that the shape of basis function tails is not analytically constrained. In practice, we use hydrogen-like basis function tails, and explicitly control their radial extent. This prescription recovers the complete basis set convergence properties of the largest available quantum chemical basis sets for perturbation theory, but with significantly smaller basis sets and numerical efficiency. [1] V. Blum, et al., Comp. Phys. Comm. 180, 2175 (2009); [2] H. Eshuis, F. Furche, J. Chem. Phys. 136, 084105 (2012).

O 58.35 Wed 18:15 Poster B1

Ordering in two dimensional amorphous atomic sheet — Takahiro Suzuki[1,2], Kiyoshi Koyanagi[1], Yasumasa Tanishiro[1,2], and •Kunio Takayanagi[1,2] — [1]Tokyo Institute of Tecnology — [2]Crest, JST

Amorphous film is an issue of nano-surface science, because the local ordering of atoms/ions determines electronic properties. We used an aberration corrected electron microscopy (AbC-EM) to find a local order/disorder of atoms/ions in amorphous thin films. An amorphous carbon mono-sheet is found to have a specific "local ordering" in the atomic sheet. Local order of metal ions in an amorphous InGaZnO film, a transparent amorphous oxide semiconductor (TAOS), is found to be seen also by AbC-EM. The electron transport via overlapping between neighboring metal s-orbitals in TAOS is discussed in terms of the local ordering.

O 58.36 Wed 18:15 Poster B1

ROSE: ROtatable Spin-polarized Electron source — •Sebastian D. Stolwijk, Henry Wortelen, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster

Surfaces of non-magnetic materials may exhibit surface states with complex spin structures in reciprocal space. To understand the fundamental mechanisms of the underlying effects, it is crucial to obtain as complete information as possible on the polarization of the electronic states. So far, current spin- and angle-resolved inverse photoemission experiments are limited to one polarization direction. Here, we introduce a recently developed **RO**tatable **S**pin-polarized **E**lectron source (ROSE). Briefly, this is based on a GaAs spin-polarized electron source, which is modified by embedding a variable rotation of the source chamber. It produces a transversally spin-polarized electron beam, whose polarization direction lies either in the plane of incidence or is perpendicular to it. With ROSE, the inverse photoemission experiment is sensitive to at least two in-plane polarization directions. Furthermore, by rotating the sample, one gains sensitivity to the out-of-plane component. In-situ measurements of the unoccupied electronic structure of Tl/Si(111) demonstrate the beauty of the ROSE.

O 58.37 Wed 18:15 Poster B1

Combined STM/AFM study on cyclic trimeric perfluoro-ortho-phenylene mercury — •Florian Albrecht[1], John McManus[1], Martin Fleischmann[2], Manfred Scheer[2], and Jascha Repp[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Inorganic Chemistry, University of Regensburg, 93053 Regensburg, Germany

Despite the fact that cyclic trimeric perfluoro-ortho-phenylene mercury (TPM) molecules have a relatively large void at their center, their lowest unoccupied molecular orbital (LUMO) was calculated to have highest density just there [1]. To verify this experimentally, we studied TPM by means of low-temperature combined scanning tunneling (STM) and atomic force microscopy (AFM). From combining the structural information obtained in the AFM with the electronic information in the STM channel, we indeed confirm this picture. The molecule has the tendency to attract electron rich ligands at its center. We directly mapped out the interaction of a prototype ligand to the TPM molecule by attaching the ligand to the tip and measuring its interaction with the molecule adsorbed on the sample surface.

[1] M. R. Haneline and F. P. Gabbai, Inorg. Chem., 44, 6248, (2005)

O 58.38 Wed 18:15 Poster B1

FIM meets AFM: Quantification of Long-Range Forces in Non-Contact Atomic Force Spectroscopy using Field Ion Microscopy Characterized Tips — •Jens Falter[1,2], Gernot Langewisch[2], Hendrik Hölscher[3], Harald Fuchs[2], and André Schirmeisen[1] — [1]Institute of Applied Physics (IAP), Justus-Liebig-University Giessen — [2]Center for Nanotechnology (CeNTech) and Institute of Physics, University of Muenster (WWU) — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe

Non-contact Atomic Force Microscopy (ncAFM) is capable to measure interaction forces between the probing tip and the sample with atomic precision. Although the sample can be imaged with atomic resolution, the structure of the tip remains unknown in most ncAFM experiments. Therefore, a quantitative comparison to models from theory is often impossible. Here we present long range ncAFM force spectroscopy experiments with FIM characterized tungsten tips on Ag(111) [1]. With the additional information about the tip geometry, the measured forces can be compared to analytical models. Our analysis shows a quantitative agreement between experiment and theory for the van der Waals- and electrostatic forces [2, 3]. Even more interestingly our approach provides a value for the absolute tip sample distance. Furthermore, an additional force contribution of long range character can be separated and assigned to arise from so called "patch charges" [4].

[1] J. Falter et al, submitted to PRB (2012) [2] S. Hudlet et al, Eur. Phys. J. B 2, 5-10 (1998) [3] C. Argento and R.H. French, J. Appl. Phys. 80 (11), (1996) [4] N.A. Burnham, Phys. Rev. Lett. 69, 1 (1992)

O 58.39 Wed 18:15 Poster B1

Dynamic Friction Force Microscopy: Imaging via control of nonlinear cantilever oscillation — •Felix Mertens, Thomas Göddenhenrich, and André Schirmeisen — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392 Gießen

A dynamic friction force microscopy technique is presented, which uses the nonlinear cantilever oscillation response to control the sample modulation amplitude. A periodic stick-slip motion of the tip at higher modulation amplitudes leads to an additional cantilever resonance frequency signal due to a self-excited cantilever oscillation. Using a lock-in amplifier together with a modulation amplitude feedback control system, friction contrast in terms of the modulation amplitude near the nonlinear-to-linear regime can be obtained. Applying this technique on HOPG, the observed friction images clearly reveal higher friction at step edges as well as an area contrast otherwise unseen in the topography.

O 58.40 Wed 18:15 Poster B1

Surface investigation of Topological Insulators with STM and STS: From local defects and aging processes. — •Sebastian Fiedler[1,2], Peter Lutz[1,2], Henriette Maas[1,2], Christoph Seibel[1,2], Hendrik Bentmann[1,2], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg, Germany — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institute für Technologie KIT, 76021 Karlsruhe, Germany

Topological Insulators (TIs) are presently one of the most promising topics in solid state physics. Theoretical calculations predict a spin polarised current on the surface of the TI without electrical resistance, which should be robust since the involved states are protected by time reversal symmetry. This dissipation-less transport of a spin polarised current requires an insulating bulk and a band gap with two crossing bands, one for spin up and one for spin down states [1]. However, defects are the main reason, why the bulk is not insulating thus destroying this effect. We investigate the surface of TIs with Scanning Tunnelling Microscopy (STM) and Spectroscopy (STS). We observe local defects and measure the local electron density, which helps understanding the influence of defects. Moreover, we demonstrate that aging of the TI results in a broadening of the band gap. This effect can also be mimicked by adsorption of alkali metals.

[1] arXiv:0801.0901v1 [cond-mat.mes-hall] 7 Jan 2008

O 58.41 Wed 18:15 Poster B1

A scanning tunneling microscope exhibiting 120 ps time resolution — •Christian Saunus, Marco Pratzer, and Markus Morgenstern — II. Physikalisches Institut B and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany

Short tunneling voltage pulses are used in a pump-probe set-up to increase the time resolution of STM measurements, thereby beating the bandwidth limit of the current preamplifier.[1] Using a home built radio frequency STM, we apply voltage pulses as short as 120 ps to the tunneling junction between tip and sample. This is verified by measuring the overlap of pump and probe visible due to the non-linearity of the I-V characteristic of the junction measured independently. Atomic resolution on HOPG is achieved in the pump-probe mode exploiting differences in the non-linearity of $I(V)$ which basically corresponds to a d^2I/dV^2 mapping on HOPG.

[1] S. Loth, M. Etzkorn, C. P. Lutz, D.M. Eigler, and A. J. Heinrich, Science **329**, 1628 (2010).

O 58.42 Wed 18:15 Poster B1

4-Tip STM Transport Measurements on Si(111)-7x7 — •Marcus Blab, Matthias Wunde, Vasily Cherepanov, Peter Coenen, and Bert Voigtländer — Forschungszentrum Jülich, Peter Grünberg Institut, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology

An ultra compact 4-tip STM was constructed in order to investigate the charge transport on the nanoscale. An n-doped Si(111)-7x7 sample was chosen as a first test sample. We will present atomic resolution images with all four tips and distance dependent 4-tip transport measurements of this surface. These measurements are compared with finite elements calculations, which show a strong tip distance dependence of the current density. Furthermore the calculations show a possibility to suppress the bulk in order to measure the surface conductance of Si(111)-7x7.

O 58.43 Wed 18:15 Poster B1

A combined LT-STM/FIM for tip specific tunnelling experiments — •Matthias Müller, Ben Wortmann, and Rolf Möller — Faculty of Physics, Center of Nanointegration Duisburg-Essen, University of Duisburg- Essen, 47048 Duisburg, Germany

We present details on a homebuilt, compact, low temperature scanning tunnelling microscope that allows in situ field ion microscopy of a cooled tunnelling tip inside the STM. Therefore a characterisation of the tip is possible without transfer to a different position in the UHV system, so that the characterised tip is identical to the one used in the STM experiment. The geometry of the microscope resembles a cylinder with a height of 13 cm and a diameter of 4 cm. The STM is screwed directly onto a commercially available continuous flow cryostat which allows cooling to about 5-7 K. The very compact design minimises helium consumption to about 1 litre/hour. Insulation from vibration is provided by a combination of springs and eddy current damping. Shutters at the bottom of the microscope can be opened to expose the tip to a channel plate or closed to assure even lower temperatures and minimal thermal drift while tunnelling. A combination of two piezo-electric accentuators is used to move a magnetically attached slider holding the tip. The slider can be easily exchanged in vacuum. The performance of the STM setup has already been shown for an almost identical system [1]. [1] (H. Karacuban, M. Lange, J. Schaffert, O. Weingart, Th. Wagner and R. Möller, Surf. Sci. Lett., 603, Issue 5, L39 (2009).

O 58.44 Wed 18:15 Poster B1

Development of a low-temperature scanning tunneling microscope for spin-polarized measurements in high magnetic fields — •Oliver Storz, Paolo Sessi, and Matthias Bode — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg

The discovery and characterization of new phenomena in surface science calls for advanced experimental techniques which combine ultra-high spatial and energy resolution with extreme environments. Here we present a new Scanning Tunneling Microscope (STM) designed for spin-polarized measurements at low temperatures and in high magnetic fields. Cooling is achieved by pressing the STM head against a pumped liquid He bath with a base temperature $T \leq 1.2\,\mathrm{K}$. A superconducting magnet supplies a vertical field up to 12.5 T. The microscope design and the materials used have been optimized to achieve high resonance frequencies, resulting in an excellent stability of the instrument. A piezo-driven x, y-sample stage allows for a lateral travel range of ±2 mm. By means of a linear transfer system the STM head can be moved between the measurement position inside the cryostat and a position for tip and sample exchange as well as for in-situ deposition onto the cold sample surface.

O 58.45 Wed 18:15 Poster B1

Atomic Resolution on KBr (100) Achieved by Means of KPFM and nc-AFM — •Timm Volkmann, Aaron Gryzia, Armin Brechling, and Ulrich Heinzmann — Molecular and Surface Physics, Bielefeld University

We modified an Omicron UHV AFM/STM for Kelvin Probe Force Microscopy (KPFM). The modified setup consists out of a nanoSurf easy PLL plus Controller/Detector for AFM, and a Signal Recovery DSP Lock-in Amplifier and SRS Analog PID Controller for KPFM. Cleaving potassium bromid (KBr) under ambient conditions and consecutive heating provides a clean surface for atomic imaging. We did research regarding different baking parameters. Annealing reduces contamination and electrostatic forces on the sample surface. Finally, cleaving the crystal in-situ provides a significant improvement of the image quality in the contact potential difference (CPD) and topography data.

O 58.46 Wed 18:15 Poster B1

Combination of Tuning Fork Non-Contact Atomic Force Microscopy with Field Ion Microscopy — •Sören Zint[1], Andreas Nejbert[1], Dirk Dietzel[1], Jens Falter[1], André Schirmeisen[1], and Harald Fuchs[2] — [1]Institute of Applied Physics (IAP), Justus-Liebig-University Giessen — [2]Center for Nanotechnology (CeNTech) and Institute of Physics, University of Muenster (WWU)

Non-contact atomic force microscopy (ncAFM) has proven to be a valuable tool for surface characterization with atomic-resolution. For a quantitative comparison between force spectroscopy experiments and corresponding analytical models, knowledge of the true tip geometry is required. One method for determining the tip geometry is the field ion microscopy (FIM) technique. Thus we combined a tuning fork sensor based low temperature AFM with the field ion microscopy technique, in one ultra-high vacuum chamber. With this AFM we can acquire atomically resolved AFM images (e.g. on NaCl) together with force spectroscopy data, while the FIM allows for tip reconstruction of electrochemical etched tungsten tips. This setup enables us now to approach the problem of correlating specific features of force spectroscopy experiments with corresponding tip geometries.

O 58.47 Wed 18:15 Poster B1

Infrared subsurface imaging of nanoparticles embedded in textile fibres — •Alfred van Munster[1,3], Benedikt Hauer[1], Benjamin Glauss[2], Wilhelm Steinmann[2], Markus Beckers[2], Thomas Gries[2], and Thomas Taubner[1,3] — [1]I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany — [2]Institut für Textiltechnik ITA, Otto-Blumenthal-Straße 1, 52074 Aachen, Germany — [3]Fraunhofer-Institut für Lasertechnik ILT, Steinbachstraße 15, 52074 Aachen, Germany

The mechanical and electrical properties of polymer based materials (e.g. fibres) are affected by additives like nanoparticles [1]. However, it is difficult to detect the location of embedded nanoparticles beneath the surface without damaging the sample. Scattering-type scanning near-field optical microscopy (s-SNOM) offers the opportunity to characterize a sample in such a non-destructive way. The evanescent field at the apex of a sharp, illuminated tip is used to probe the dielectric properties of a material with a sub-wavelength resolution given by the tip radius.

In our sample system siliconcarbide nanoparticles are embedded in polypropylene fibres. At mid-infrared wavelengths the phonon polaritons in SiC resonantly enhance the near-field interaction [2]. We compare the experimental data to reference measurements on bulk SiC and to the calculated predictions of a layered system model [3].

[1] W. Steinmann et al., Text. Res. J. 82, 1846 (2012).

[2] R. Hillenbrand et al., Nature 418, 159 (2002).

[3] B. Hauer et al., Opt. Express 12, 13175 (2012).

O 58.48 Wed 18:15 Poster B1

The detection of light emitted from the tunneling junction of a low temperature STM — •Ebru Özen, Maren C. Cottin, Johannes Schaffert, Rolf Möller, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

The decrease in size of the building blocks used in modern electronic devices requires the understanding of electronic transport phenomena down to the atomic level. Beside the elastic tunneling processes in a scanning tunneling microscope (STM) experiment, also inelastic processes take place. This leads to an excitation of the sample. The relaxation may decay e.g. by emission of photons [1]. The spectral analysis of the emitted light from the tunneling junction in the STM experiment provides valuable information about radiative decay channels, e.g. within an adsorbed organic molecule [2]. We implemented an experimental setup for the detection of photons which are emitted during the decay of the excitation of the sample. During first measurements light from the tunneling junction either during field emission or tunneling could efficiently be detected.

[1] R. Berndt et al., Science 262, 1425 (1993). [2] C. Chen et al., Phys. Rev,. Lett. 105, 217402 (2010).

O 58.49 Wed 18:15 Poster B1

Study of protein DNA interaction by simultaneous atomic force and fluorescence microscopy — •Sören Grannemann, Volker Walhorn, and Dario Anselmetti — Bielefeld University, Bielefeld, Germany

Atomic force microscopy (AFM) and fluorescence microscopy are in each case valuable tools for affinity studies at the single molecule level. A combination of both might even provide further insights in intermolecular binding and dissociation processes.

We combined AFM with total internal reflection microscopy (TIRFM) to study the affinity of a fluorescently labeled Protein DNA receptor ligand pair. The fluorescence markers were chosen such that Fluorescence Resonant Energy Transfer (FRET) can occur at close proximity of the dye molecules. Consequently, receptor-ligand binding should be correlated with FRET.

In first proof of principle experiments we used the DNA-binding Domain of the transcriptionfactor PhoB from *E.coli* and the associated DNA containing the PhoB recognition sequence as receptor-ligand system. Simultaneously acquired force and acceptor fluorescence data showed a correlation between the decrease of acceptor fluorescence intensity and molecular dissociation events of the Protein-DNA complexes. In present experiments, the donor fluorescence is measured additionally to prove the anti-correlation of donor and acceptor fluorescence intensity as well.

O 58.50 Wed 18:15 Poster B1

A simple design to convert an UHV-STM into an AFM — •Stefan Borgsdorf and Ulrich Köhler — Experimentalphysik IV, Ruhr-Universität Bochum, Germany

A simple design of an atomic force microscope (AFM) is presented, by which an ultra high vacuum scanning tunneling microscope (UHV-STM) is converted into an UHV-AFM. For this purpose piezoresistive Cantilevers with bimorph actuator are used. Under these conditions it is less complicated to build up an AFM in vacuum than with an optical readout. In our setup the cantilever is scanning. Therefore the tip is located in the middle of the piezo tube to minimize the crosstalk between different scanning directions as in STM. Another requirement is that it should be able to exchange the sensor in the vacuum chamber and also to create a layout to exchange the sensor type, for example to a qPlus Sensor.

O 58.51 Wed 18:15 Poster B1

Nanosecond scanning tunneling microscopy — •Shichao Yan[1,2], Deung-Jang Choi[1,2], and Sebastian Loth[1,2] — [1]Max Planck Research Group-Dynamics of Nanoelectronic Systems, Center for Free-Electron Laser Science, Hamburg — [2]Max Planck Institute for Solid State Research, Stuttgart

The scanning tunneling microscope (STM) can provide very high spatial resolution down to the atomic scale. One of the usual limits of the STM technique is its limited time resolution which is typically miliseconds because of the bandwidth of the control electronics. Yet, many processes on the nanoscale occur at nanosecond speed or faster. We present the instrumentation and test of a scanning tunneling microscope system that combines sub-Kelvin operation with high-frequency electronic circuitry. Nanosecond or picosecond electric pump-probe pulses can be introduced into the tunneling junction with high fidelity to study the dynamics of the nanostructures. The design of the high bandwidth circuitry and the cooling mechanism of the semi-rigid cables will be presented. With this instrument, we have reached nanosecond time resolution while maintaining atomic spatial resolution. We apply this technique to measure the spin relaxation time of iron nanostructures on copper nitride. In principle, the electric pump-probe STM technique can also be used to study long lifetime vibrational excitations and conformational changes of molecules.

O 58.52 Wed 18:15 Poster B1

Investigation of single Co atoms on Mn/W(001) — •Arne Köhler, Alexander Schwarz, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Germany

Recently, the magnetic coupling between single Co atoms and the antiferromagnetic spin-spiral of Mn/W(110) has been studied with Scanning Tunneling Microscopy [1]. Using the ferromagnetic spin-spiral of Mn/W(001) [2] as a further complex magnetic template for Co atoms, our final goal is to investigate local magnetic properties of Co adatoms using Magnetic Exchange Force Microscopy [3] and Spectroscopy [4].

To inhibit aggregation of Co atoms on the substrate, they are deposited and investigated at low temperature. In our particular set-up, Co atoms are deposited from a miniature evaporator inserted into the cantilever holder. After deposition, different atomic scale contrast features are found on the substrate, indicating several adsorbed species. The origin of these adsorbates can be twofold: coadsorption during Co evaporation, i.e., CO, or formation on the surface after deposition, i.e., H:Co complexes. The latter is of particular interest, as it can be expected that H:Co behave magnetically different than single Co atoms.

Therefore, it is necessary to differentiate between Co atoms and other species on the surface.

[1] D. Serrate et al., Nat. Nanotech. 5, 350 (2010).
[2] P. Ferriani et al., Phys. Rev. Lett. 101, 027201 (2008).
[3] U. Kaiser et al., Nature 446, 522 (2007).
[4] R. Schmidt et al., Phys. Rev. Lett. 106, 257202 (2011).

O 58.53 Wed 18:15 Poster B1

Heat transfer through a single molecule — •Nils Könne, Ludwig Worbes, David Hellmann, Konstantin Kloppstech, and Achim Kittel — EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg

The measurement of the molecular heat transfer at the single molecule level has attracted a lot of interest in recent years [1]. To measure this phenomenon with high spatial resolution we use our self-developed near field scanning thermal microscope (NSThM). Hence we are able to simultaneously detect the electron and heat transfer through a single molecule under ultra-high vacuum conditions. The conductions measurements are done for different temperature and potential differences within an Au-octanedithiol-Au junction using the NSThM-break junction technique. We have proven our concept by repeatedly retract the tip from the octanedithiol covered surface and record the distance dependency of the conductance which partially exhibit a step like behaviour. The histogram of these conduction steps reveals the commonly known [2] low conduction value of 1 nS for a single octanedithiol. [1] Yonatan Dubi and Massimiliano Di Ventra, Rev. Mod. Phys. 83, 131 (2011). [2] Wolfgang Haiss et al, J. Phys. Chem. C 113, 5823-5833 (2009).

O 58.54 Wed 18:15 Poster B1

In situ characterization of thermal resistance of sensor tips of a near-field scanning thermal microscope (NSThM) — •Konstantin Kloppstech, Nils Könne, Ludwig Worbes, and Achim Kittel — EHF, Inst. f. Physik,CvO Universität Oldenburg

The experimental analysis of near-field heat transfer by means of absolute fluxes is based on accurate knowledge of the thermal resistance of the thermocouple sensor. We present an accurate in situ method for the determination of the sensor's thermal resistance which can be applied for each sensor right before the scanning procedure. Therefore a sample holder consisting of a 5μm thin and 3-10mm long tungsten wire which is glued to an isolated copper block is realized. The wire itself is mechanically pre-tensioned to minimize thermal vibrations because it is heated via a high frequency current. By this a temperature profile will develop along the wire resulting in a measurable change in electric resistance. Parasitic heat-drain channels can be neglected, because the experiment is performed in UHV. The determination of the thermal resistance of the tip is performed in two steps. First, the mean temperature rise is calculated for various values of heating power. Thermal resistance of the wire is determined by fitting the curve of temperature change versus heating power. Second, the tip is being approached to the wire resulting in a second channel for heat drain. The thermal resistance of the tip is then calculated from the resulting temperature change for different heating powers of the coupled system. This can be done by means of solving a 1d heat transfer equation, which describes the coupled systems of wire and tip.

O 58.55 Wed 18:15 Poster B1

Highly controlled electron bombardment of SPM-tips for cleaning — David Hellmann, Ludwig Worbes, Konstantin Kloppstech, Nils Könne, and •Achim Kittel — EHF, Faculty V, Department of Physics, C. v. O. University of Oldenburg, 26129 Oldenburg, Germany

In the field of scanning probe microscopy, it is of great importance to operate with a well defined state of sample and probe with respect to unintentionally adsorbed molecules. There are many techniques for tip cleaning described in literature; among others the use of accelerated electrons as an energy source is reported. So far, all of the setups described, yielded either no or only indirect information about the probe's temperature reached during the cleaning procedure, which is an important quantity to control the process. The Near-Field Scanning Thermal Microscopy probe not only serves as scanning tunneling microscope tip, but also includes a thermosensor in the vicinity of the probe's apex. These sensors are very delicate because they combine different kind of materials. We use electron bombardment for cleaning these unique sensors, while the thermosensor is used as a sensor in the loop which is controlling the procedure. We observed probe temperatures up to 1800 K for a few tens of milliseconds without causing any damage to the tip function. We describe here the device as well as experimental data concerning the relation between the energies used for cleaning and the resulting temperature of the probe. The presented data might serve as an indicator for other setups where a direct measurement of the temperature of the apex is impossible.

O 58.56 Wed 18:15 Poster B1

Fabrication of gold nanocone near-field scanning microscope probes — •Omar Tanirah[1], Alexander Weber-Bargioni[2], Stefano Cabrini[2], Dieter P. Kern[1], and Monika Fleisher[1] — [1]Institute for Applied Physics, Eberhard Karls University Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Molecular Foundry, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, California 94720, United States

Gold nanostructures have fascinating plasmonic properties. Hence, they are promising for a vast field of cutting edge nanophotonics technology. Our special interest is focused on developing near-field scanning optical microscopy (NSOM) probes by combining scanning probes with gold nanostructures. NSOM probes with plasmonic nanocones are expected to enable simultaneously ultrahigh resolution spectroscopy and topography measurements [1]. This is possible since the nanocone has an outstanding shape which can restrict the localized surface plasmon to subwavelength dimensions. Here, we report the fabrication of gold nanocones on top of both atomic force microscope (AFM) cantilevers and optical fibre tips. The fabrication method depends mainly on focused ion beam, electron beam induced deposition, and ion milling techniques. This method provides precise control over size and shape of the gold nanocones, and accordingly their plasmonic properties. Their optical properties were investigated by means of dark field spectroscopy, and their morphology was studied using AFM and scanning electron microscopy. Results of both fabrication and characterization will be shown. [1] M. Fleischer et al., ACS Nano 5, 2570 (2011).

O 58.57 Wed 18:15 Poster B1

Enhanced heat transfer by nanoscale NaCl-Islands on Au(111) observed by Near-field Scanning Thermal Microscopy (NSThM) — •Ludwig Worbes, David Hellmann, Konstantin Kloppstech, Nils Könne, and Achim Kittel — EHF, Faculty V, Department of Physics, C. v. O. University of Oldenburg, 26129 Oldenburg, Germany

Due to the advance in nanoscience heat transport at small length scales is receiving more attention as a field of fundamental research as well as one influencing future technologies. The Near-field Scanning Thermal Microscope (NSThM) is a tool to investigate heat transport on the nanoscale[1]. It is based on a UHV-STM, featuring a tunneling probe with an integrated miniaturized thermocouple temperature sensor. Therefore, we can measure the temperature change of the tip due to heat flux between a heated or cooled sample and the probe in the range of distances between (tunnel-) contact and a few nanometers with high spatial resolution.

In this poster we present measurements of the heat-flow above one monolayer thick islands of NaCl prepared by physical vapor deposition on top of Au(111). We observe a distinct enhancement due to the NaCl-layer. For future applications such measurements are important for designing the heat flow management of nanoscaled devices. Such measurements may also trigger new theoretical approaches, because they show a distinct effect at length scales below the ones described by the established macroscopic theories.

[1] Uli F. Wischnath et al., Rev. Sci. Instrum. 79, 073708 (2008)

O 58.58 Wed 18:15 Poster B1

Measurements of elastic properties of surfaces with nanometer resolution — •Marina Sarmanova, Erik Thelander, Alexander Malwin Jakob, Jürgen W. Gerlach, Stefan G. Mayr, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, D-04318 Leipzig

Quantitative and qualitative measurements of local mechanical properties on nano and ultra-fine scale are useful for both fundamental research of physical properties of the surface and quality control of modern nano-scale devices. The experimental arrangement of mechanical measurements with nanometer resolution is demonstrated. Measurements of Young's modulus of surfaces could be performed with high resolution by means of contact resonance force microscopy (CR-FM) [1]. It is shown that CR-FM technique is suitable for measurements of materials with Young's modulus in a wide range. The local elastic properties of Ge2Sb2Te5, a phase change material well known for its data storage application based on the well-pronounced difference of optical and electrical properties between amorphous and crystalline phases, were investigated. GaN, a semiconductor with wide band-gap, famous for production of high-efficiency diodes and lasers, yields high values of local Young's modulus. This project is funded by Leibniz Association. [1] Rabe U., Arnold W., Appl. Phys. Lett. Vol.64, P1493-1495 (1994)

O 58.59 Wed 18:15 Poster B1

Time of Flight X-Ray Photoelectron Spectroscopy — •Stephan Hannig[1], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]E1-TU Dortmund, Otto-Hahn-Straße 4, D-44227, Germany — [2]DELTA-TU Dortmund, Maria-Goeppert-Mayer-Straße 2, D-44227, Germany

X-ray Photoelectron Spectroscopy (PES) reveals the electronic structure of surfaces by detecting the energy distribution of short mean-free path photo-emitted electrons. Conventional setups consist of a channeltron-detector attached to a concentric hemispherical analyzer. A disadvantage of this technique is the limited lifetime of the electron multiplier inside the detector. In addition to that, measurements are rather time-consuming if large angle scans have to be performed as in photoelectron diffraction experiments. Here we present the first tests of the applicability of a delay-line detector at the synchrotron DELTA and its performance. In the next step the setup will be compared to the existing conventional detector described above.

O 58.60 Wed 18:15 Poster B1

Fully Controlled, High Flux Electrospray Ion Beam Deposition of Nonvoaltile Molecules in Vacuum — •Stephan Rauschenbach[1], Gordon Rinke[1], Matthias Pauly[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Institut Physique de Matière Condensée, École Polytechnique Fédéral de Lausanne, Switzerland

The inherent chemical purity and the ability to control the growth make vapor deposition in vacuum an extremely successful technology with applications from food packaging to semiconductor devices. Large functional molecules of either natural or synthetic origin, however, tend to be thermally labile, which hinders the conventional vacuum processing by evaporation. Alternative approaches to evaporation often do not reach the performance of vapor deposition in vacuum terms of purity, control, versatility, or deposition rate.

We developed electrospray ion beam deposition (ES-IBD) as a method for the vacuum deposition of non-volatile molecules. ES-IBD is based on electrospray ionization, a soft ambient ionization method, creating intact molecular gas phase ions of even fragile molecules. The deposition apparatus is differentially pumped and contains ion optics in each stage, conveying the ion beam to the target in UHV, as well as current detectors and mass spectrometers, together providing full control over the deposition process. In addition our newly designed, hydrodynamically optimized electrospray ion source provides high flux and high efficiency, which demonstrates the potential of ES-IBD for commercial applications.

O 58.61 Wed 18:15 Poster B1

Fast XPS - monitoring surface reactions in the microsecond regime — •Oliver Höfert, Max Amende, Stefan Schernich, Christoph Gleichweit, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

High temperatures and low coverages are hard to handle in reaction studies under surface science conditions and the respective analytical methods, due to the short characteristic reactions timescales. In this study, we show that by improving the time resolution of photoelectron spectroscopy, we can follow surface reactions at high temperatures in the microsecond regime. This is realized by recording the signal at selected (and characteristic) binding energies as function of time. By using a periodic dosing procedure and subsequent adding up of the resulting data sufficient signal to noise ratio is obtained. Further improvements towards an even better time resolution are envisioned. As a first test case the adsorption and desorption of CO on Pt(111) was studied at temperatures between 460 K and 500 K with a time resolution of 500 μs. The experiments have been performed at the synchrotron facility BESSY II.

This work was supported by BMBF (05 ES3XBA/5) and the DFG through the Cluster of Excellence "Engineering of Advanced Materials".

O 58.62 Wed 18:15 Poster B1

Characterization of an Effusive High Flux Metal Source — Han Zhou, Benedikt Klein, Hans-Jörg Drescher, and •J.Michael Gottfried — Philipps-Universität, Marburg

The here presented pulsed molecular / atomic beam source and signal detector are designed for Nanojoule Adsorption Calorimetry (NAC), which is a technique especially suitable for the characterization of non-reversible molecular or atomic adsorption enthalpies on well defined substrates in ultrahigh vacuum. Similar to previous adsorption calorimeters by Černy, King and Campbell, NAC relies on the direct measurement of mircoscopic temperature changes induced by incremental adsorption utilizing pyroelectric detectors. NAC requires long-term stable fluxes at high evaporation rates leading to special requirements on the deposition source, e.g. high volume and constant evaporation temperature established by specially designed evaporator with relatively higher capability of heat generation and proportional-integral-derivative controlling which enables sensitive and non-linear evaporator self-administration. Inspired by the investigations on interfaces between low work-function metals and semi-conducting organic molecules, we here present the characterization of the evaporator regarding the most important parameters as well as the performance of additional pulse-defining devices using Magnesium as adsorbate. In addition the degrading, i.e. the loss of sensitivity, of the pyroelectric detectors due to thermal exposure during bake-outs and the effect of corresponding compensation techniques, i.e. electrical inducement during thermal treatment, were systematically studied.

O 58.63 Wed 18:15 Poster B1

Characterization of an Effusive High Flux Metal Source and of Pyroelectric Detectors for Nanojoule Adsorption Calorimetry — •Han Zhou, Benedikt Klein, Hans-Jörg Drescher, and J. Michael Gottfried — Fachbereich Chemie, Physikalische Chemie, Philipps-Universität Marburg, 35032 Marburg, Hans-Meerwein-Str.

The here presented pulsed molecular / atomic beam source and signal detector are designed for Nanojoule Adsorption Calorimetry (NAC), which is a technique especially suitable for the measurement of non-reversible molecular or atomic adsorption enthalpies on well defined substrates in ultrahigh vacuum. Similar to previous adsorption calorimeters by Černy, King and Campbell, NAC utilizes pyroelectric detectors for the direct measurement of temperature changes in the μK range induced by incremental adsorption. NAC requires long-term stable fluxes at high evaporation rates leading to special requirements on the deposition source, e.g., high volume and constant evaporation temperature established by proportional-integral-derivative controlling. Motivated by the general interest in interfaces between low work-function metals and semi-conducting organic molecules, we here present the characterization of the evaporator regarding the most important parameters as well as the performance of additional pulse-defining devices using Magnesium as an adsorbate. In addition, the sensitivity of the pyroelectric detectors and its dependence on thermal stress and other factors are systematically studied.

O 58.64 Wed 18:15 Poster B1

Surface segregation of FePt investigated by STM, XPS and PAES — •Samantha Zimnik[1], Christoph Hugenschmidt[1,2], and Florian Lippert[1] — [1]TU München, Lehrstuhl E21, James-Franck Straße, 85748 Garching — [2]ZWE FRM-II, Lichtenbergstr. 1, 85747 Garching

Segregation processes are of high importance for the understanding of the macroscopic properties of thin films or nano particles such as the magnetization in the system FePt. Positron annihilation induced Auger Electron Spectroscopy (PAES) is a powerful technique to gather information about the elemental composition of only the topmost atomic layer of a sample. Time dependent PAES allows the observation of the segregation process in-situ. The results are compared with X-ray induced Photoelectron Spectra (XPS). The Scanning Tunneling Microscope (STM) is used as a complementary method to investigate the electron density with atomic resolution of the same sample before and after the segregation process. PAES, XPS and STM allow the characterization of both, the elemental composition and the surface topology. The new experimental setup at NEPOMUC at the FRMII in Munich enables the preparation as well as the characterization of the sample using PAES, XPS and STM. Financial support within the project no. 05KI0WOB by the BMBF is gratefully acknowledged.

O 58.65 Wed 18:15 Poster B1

Combining High-Resolution Scanning Probe Studies with Re-

activity Experiments — •Hendrik Ronneburg, Stefanie Stuckenholz, Christin Büchner, Gero Thielsch, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

In our group we use noncontact atomic force microscopy (nc-AFM) and scanning tunneling microscopy (STM) for the analysis of metal supported thin oxide films. This custom built instrumentation gives us the opportunity to gain a deeper understanding of oxide surfaces at the atomic level, e.g. MgO [1].

These scanning probe measurements should ideally be accompanied by reactivity studies. Therefore, we are setting up a new temperature programmed desorption (TPD) experiment.

In this setup the adsorption of CO on MgO surfaces will be studied. This reaction serves as a model for the interaction of CO with an ionic surface [2, 3].

Plans for the integration of a low temperature TPD setup with the existing ultra high vacuum chamber will be presented.

[1] T. König, *et al.*, Beilstein J. Nanotechnol. **2**, 1 (2011)
[2] R. Wichtendahl, *et al.*, Phys. Status Solidi A **173**, 93 (1999)
[3] M. Sterrer, *et al.*, Surf. Sci. **596**, 222 (2005)

O 58.66 Wed 18:15 Poster B1

Helium Ion Microscopy as tool to investigate thin layer thicknesses — •Henning Vieker, Karsten Rott, Udo Werner, André Beyer, Günter Reiss, and Armin Gölzhäuser — Bielefeld University, Faculty of Physics, Germany

The recently developed helium-ion microscope allows remarkable surface resolution with the secondary-electron (SE) detector. Simultaneously, backscattered ions can be detected that allow imaging with a substantially higher elemental contrast. This Rutherford backscattered ion (RBI) contrast depends mainly on the elemental composition of the investigated sample surface. The escape depth of backscattered ions is much larger than for secondary electrons. Thus whole layers with a wide range of thicknesses will contribute to a RBI image, whereas the SE image is far more surface sensitive, i.e. insensitive to buried parts under the sample surface.

In this contribution we examine RBI imaging as tool to characterize thickness variations of layered samples with well defined compositions. In a model example the homogeneity of gold layers on silicon substrates is investigated and compared to simulation data. Achievable spatial resolutions as well as the possibilities in using a reference sample to measure layer thicknesses will be addressed. Furthermore, buried layers are investigated.

O 58.67 Wed 18:15 Poster B1

Angular and Energy Resolved Measurement of Reemitted Positrons from W, Pt and Ni Single Crystals — •Florian Lippert[1], Samantha Zimnik[1], Hubert Ceeh[1], Christian Piochacz[2], and Christoph Hugenschmidt[1,2] — [1]TU München, Physik Department, Lehrstuhl E21, James-Franck-Str. 1, 85748 Garching — [2]TU München, FRM II, Lichtenbergstr. 1, 85748 Garching

Monoenergetic positron beams are applied for a variety of non-destructive experiments in surface- and solid state physics. In order to create monoenergetic positrons, so called (re-)moderating materials with negative positron work functions are used, such as W, Pt and Ni. After thermalisation and diffusion to the surface, moderated positrons leave the solid with an energy according to the absolute value of the positron work function. In this work the angular distribution of reemitted positrons from W(100), W(110), Pt(100), Pt(110), Ni(100) and Ni(110) is being measured. In addition, low-temperature measurements are performed to study the thermal spread. Financial support within the project no. 05KI0WOB by the BMBF is gratefully acknowledged.

O 58.68 Wed 18:15 Poster B1

Effects of electron-phonon coupling on excitation spectra — •Honghui Shang, Christian Carbogno, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

The electron-phonon interaction plays a crucial role in many areas of physics. The main purpose of our study is to investigate the effect of the electron-phonon coupling on the excitation spectra of (organic) molecules and solids. For example, the phonon induced renormalization of electronic excitations can be as large as a few tenths of an eV for diamond and similar magnitudes are expected for other materials such as SiC, GaN, ZnO. To incorporate electron-phonon effects from first principles we employ a Green function/self-energy framework. Here we present an implementation for the electron-phonon coupling matrix elements in the all-electron Fritz Haber Institut *ab initio* molecular simulations (FHI-aims) package [1]. For the calculations of the first-order density response, both the coupled-perturbed self-consistent field method and density functional perturbation theory have been implemented. By comparing with the results from finite differences, the accuracy of the first-order response in the Hamiltonian and the density is demonstrated for both methods. With the first-order density response, the electron-phonon coupling matrix elements are then calculated using numeric atom-centered orbital (NAO) basis sets. Due to the spatial locality of the NAO basis set, we anticipate our approach be applicable to large systems up to hundreds of atoms.

[1] https://aimsclub.fhi-berlin.mpg.de/

O 58.69 Wed 18:15 Poster B1

Monte Carlo simulations of growth processes on prepatterned surfaces — •Oleg Buller and Andreas Heuer — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster

The creation of desired structures after molecule deposition processes on prepatterned surfaces by using self-organization is a developing technique. Experiments with deposited organic molecules on prepatterned geometries display a multitude of different growth mechanisms. Here we use lattice Monte Carlo simulations to study the growth behavior in dependence of the interaction strength, the initial properties of the prepatterned surface as well as the chosen flux. It turns out that in particular the chosen interaction strength is of crucial importance for the characterization of the resulting structure.

O 58.70 Wed 18:15 Poster B1

Evaporation of nanosized droplets on heated substrates — •Jianguo Zhang, Frederic Leory, and Florian Müller-Plathe — Theoretical Physical Chemistry,Technische Universität Darmstadt , Germany

The evaporation of nanometer scale droplets (about 10 nm in diameter) on flat heated substrates has been studied. The systems were modeled by means of Lennard-Jones potentials. The interaction between the liquid and the substrate atoms was varied to reproduce a range of equilibrium contact angles from 120 to 60 degrees. The evaporation process in a closed fixed volume was followed in terms of time variations of the contact angle. It was observed that the contact angle is a monotonic decreasing function of time. However, for large equilibrium contact angles (weak solid-liquid interactions), the respective time decays are characterized by larger characteristic times than for small contact angles (strong solid-liquid interactions). The evaporation has also been characterized with spatial resolution. It was observed that the evaporation process preferentially occurs in the vicinity the three-phase contact line in the case of weak solid-liquid interactions. This observation is more contrasted in the case of the strongest solid-liquid interactions.

O 58.71 Wed 18:15 Poster B1

Representation of the 42-dimensional DFT Potential-Energy Surface of R,R-Tartaric Acid by Neural Networks — •Sinja Klees and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

The development of accurate interatomic potentials is a prerequisite to study complex systems, but often several physical approximations are indispensable to reduce the computational costs. Neural Networks (NNs) are a class of flexible mathematical functions, which allow to construct accurate interatomic potentials for systems with an arbitrary number of atoms without the introduction of any constraints on the functional form. Instead, a systematic construction of the potential-energy surface (PES) is carried out by interpolation of energies and forces obtained from first-principles reference calculations. To date, most NN PESs refer to inorganic solids and molecules up to six atom. We use R,R-Tartaric Acid to demonstrate that the method is equally applicable to organic molecules. We show that the PESs obtained from DFT reference calculations and NN interpolation are in a very good agreement.

O 58.72 Wed 18:15 Poster B1

Kondo effects in inelastic spin transitions — •Richard Korytár[1], Nicolás Lorente[2], and Jean-Pierre Gauyacq[3] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie, Germany — [2]Centro de investigación en nanociencia y nanotecnología

CIN2, Barcelona, Spain — [3]Institut de Sciences Moléculaires d'Orsay, Unité Mixte CNRS-Université, Orsay, France

Electron currents can induce magnetic excitations in molecular nanostructures. Magnetic inelastic electron tunneling spectroscopy (IETS) shows sharp increases in conductance when a magnetic excitation is induced by the incident electron. A previous one-electron theory successfully explained both the conductance thresholds and the magnitude of the conductance variation. The elastic spin flip of conduction electrons by a magnetic impurity leads to the well known Kondo effect. In the present work, we compare the theoretical predictions for inelastic magnetic tunneling obtained with a one-electron approach and with a many-body theory including Kondo-like phenomena. We apply our theories to a singlet-triplet transition model system that contains most of the characteristics revealed in magnetic IETS. We use two self-consistent treatments (non- crossing approximation and self-consistent ladder approximation). One of the main findings is that many-body effects translate into sharp peaks that appear close to the inelastic thresholds; the peaks being more robust than the Kondo resonance. Another consequence of the interaction with underlying electron gas is the reduction of the inelastic gap. This may render more difficult the extraction of magnetic anisotropy features for IETS experiments.

O 58.73 Wed 18:15 Poster B1

Electronic transport in carbon nanotubes: the role of water and long-range electrostatics — •Robert A. Bell[1], Arash Mostofi[2], and Mike Payne[1] — [1]TCM Group, Cavendish Laboratory, University of Cambridge, UK — [2]Dept. of Materials & the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, UK

Understanding interactions between carbon nanotubes and environmental adsorbants is vital for the use of nanotube devices under ambient conditions. Previous theoretical studies have concluded water n-dopes the nanotube, providing a mechanism to increase conductivity.

In this work, we show that the use of short nanotube supercells in these calculations is inappropriate in the presence of long-range electrostatic interactions. Using large-scale DFT calculations with ONETEP, we study long (>60 Å) nanotube segments, and conclude that negligible charge is transferred between the water and the nanotube. Weak long-range charge-redistribution in the nanotube is observed, however, which is explained using a simple classical electrostatic model for the polarisation of the nanotube by the water dipole. Conclusions derived from local charge transfer methods such as Mulliken analyses are unable to capture this behaviour and are potentially misleading.

Electron transport calculations, using the Landauer-Büttiker approach, on large nanotube segments with many adsorbed water molecules show only weak scattering at the nanotube valence band edge. No evidence is observed to support an increase in conductivity.

O 58.74 Wed 18:15 Poster B1

HSE06 and G_0W_0 for Pyrite- and Marcasite-type compounds — •Timo Schena, Pengxiang Xu, Martin Schlipf, Gustav Bihlmayer, Markus Betzinger, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

The accuracy of density functional theory (DFT) depends only on the choice of a suitable approximation for the *xc*-functional. The local *xc*-functionals LDA and PBE can result in a severe underestimation of band gaps in insulators and semiconductors. The prediction of the band gap is usually improved considerably by employing hybrid functionals (*e.g.* HSE06) or many-body-perturbation-theory (*e.g.* G_0W_0). Recently, these methods have been implemented in the Jülich-all-electron DFT code `FLEUR` [1,2]. However, in this work we present material systems, for which no considerable improvement of the band gaps is obtained in comparison to the experimental values. In opposite sometimes even a worsening is found. Amongst others, we present a detailed analysis of the electronic structure of Pyrite-like compounds FeS_2, RuS_2, OsS_2, NiP_2 and Marcasite-type compounds FeS_2, $FeSe_2$, $FeTe_2$ and $CrCl_2$. By detecting similarities and differences, we can draw some hypotheses of what is causing the shortcomings of HSE06 and G_0W_0 for these systems. We gratefully acknowledge funding from BMBF of the NADNuM project 03SF0402A.

[1] www.judft.de, [2] C. Friedrich *et al.* JPCM 24 293201 (2012)

O 58.75 Wed 18:15 Poster B1

Representing Complex Potential Energy Surfaces by Artificial Neural Networks — •Christopher Handley, Tobias Morawietz, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Simulations of large systems using ab initio methods are computationally costly, and in many cases intractable. An alternative is approximate interatomic potentials. These potentials are typically constructed from computationally simple functions, chosen to be representative of particular atomic interactions. Fitting of these potentials is not straightforward, as many different selections of functions and their parameters are valid, with varying accuracy. Neural Networks (NNs) recently have been shown to provide interatomic potentials that are comparable to the accuracy of quantum mechanical calculations[1,2]. NNs are flexible enough to fit complex functions, interpolating, from quantum mechanical training data, accurate energies and forces. A major drawback of the method is the non-physical functional form of the NNs. Here, we present the first steps towards a more transferable NN based upon electronic structure methods.

[1] C. M. Handley and P. L. A. Poplier, J. Phys. Chem. A, 114, 3371-3383, (2010).

[2] J. Behler, PCCP, 13, 17901-18232 (2011).

O 58.76 Wed 18:15 Poster B1

Bandgap Engineering of Layered Perovskites for Single- and Two-Photon Water Splitting — •Ivano Castelli, Kristian Thygesen, and Karsten Jacobsen — Department of Physics, Technical University of Denmark, Kgs. Lyngby, Denmark

The conversion of solar light into electrons and holes and the subsequent use of their energy to create fuels like hydrogen is one of the possible ways to address the world's pressing energy supply and storage problem. The properties determining the usefulness of a material to be used as light harvester in a photochemical cell include a narrow band gap well positioned with respect to the redox potentials of water and chemical/structural stability.

We have recently screened for one- and two-photon water splitting materials[1,2] in the cubic perovskite structure. We have found 20 promising materials for one-photon water splitting and an additional 12 for the two-photon process. We have applied the screening procedure to the double perovskite oxides and we have extracted some rules to combine two materials for obtaining a bandgap in the desired region.

We currently investigate the layered perovskite structure, consisting of 2D slabs of cubic perovskite separated by some motif, with a general formula of $A_{n-1}B_nO_{3n+1}$. We focus on finding new combinations for one- and two-photon water splitting and on designing new rules to tune the bandgap by changing the interlayer motif.

References [1] I.E. Castelli, et al., Energy Environ. Sci., 5, 5814 (2012). [2] I.E. Castelli, et al., Energy Environ. Sci., 5, 9034 (2012).

O 58.77 Wed 18:15 Poster B1

Benchmarking G_0W_0 for small metal clusters using exact frequency treatment — •Ferdinand Kaplan[1], Michiel van Setten[1], and Ferdinand Evers[2] — [1]Institute of Nanotechnoloy, Karlsruhe Institute of Technology, Germany — [2]Institute of Theoretical Condensed Matter, Karlsruhe Institute of Technology, Germany

One of the most used approaches for the computational study of solids, nanoscale systems and molecules is the density functional theory (DFT). However, as is well known, DFT calculations of single particle excitation spectra, e.g. ionization potentials and electron affinities, often suffer from approximations in exchange correlations potentials. More importantly, even fundamental difficulties exist with the common practice to identify the Kohn-Sham particles of ground-state DFT with the genuine quasi-particles.

To systematically improve the estimation of quasi-particle energies for molecular system, we have implemented the so called GW method into a standard quantum chemistry package (G_0W_0-level). The approach represents a perturbative expansion of the many-body Green's function with respect to the screened interaction, W.

Here, we present applications of the method to small metal cluster systems. First, we show that our implementation works well also in the metallic case where the HOMO-LUMO gap is relatively small, so that one might expect problems for standard perturbative results. Second, we find that deviations from experimental ionization potentials and electron affinities can be reduced against those of Kohn Sham-DFT using PBE functionals.

O 58.78 Wed 18:15 Poster B1

Quasiparticle Spectra from Self-Consistent *GW* Calcula-

tions for Transition-Metal Monoxides — •Merzuk Kaltak and Georg Kresse — University of Vienna, Computational Physics, Vienna, Austria

We present calculations for the transition-metal monoxides MnO, FeO, CoO and NiO within the framework of many-body pertubation theory, specifically using a self-consistent GW approximation with vertex corrections. Using a maximally localized Wannier projection, the band structure seems to be predicted reasonably well in the antiferromagnetic phase AFII at $T = 0$. The stacking of ferromagnetic planes in the [111] direction causes a reduction of the symmetry, which consequently leads to a splitting of the t_{2g} bands into a_g and energetically more favourable e_g states. We show that self-consistent GW quasiparticle band gaps are closer to experiment than previously published results obtained from conventional ab-initio methods using a nonlocal exchange-correlation functional with a subsequent not self-consistent G_0W_0 calculation. In addition to the electronic structure we investigate the optical properties of the compounds. To this end, the Bethe-Salpeter equation in the independent particle picture for the irreducible polarizability is solved and the optical spectrum is calculated.

O 58.79 Wed 18:15 Poster B1

A self-consistent dynamical embedding — •Wael Chibani, Xinguo Ren, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present an embedding scheme that facilitates the treatment of the physically important part of a system with electronic structure methods, that are typically computationally too expensive for periodic systems, whereas the rest of the periodic system is treated with computationally less demanding approaches in a self-consistent manner. Our embedding scheme is based on Green functions within the concept of dynamical mean-field theory (DMFT) [1] and allows the embedded region to exchange particles with its environment, a feature that distinguishes the current approach from conventional embedding schemes. In contrast with the original DMFT formulation for correlated model Hamiltonians, we consider here the unit cell as embedded cluster in an *ab initio* way, that includes all electronic degrees of freedoms. We implemented our scheme in the all-electron code FHI-aims [2]. To demonstrate the performance of the scheme we first stay within density functional theory and treat the embedded region with hybrid functionals and the environment with generalized gradient approximations, although in principle any Green functions method can be used. Preliminary tests for simple solids show that the total energy and the density of states converge well with respect to the computational parameters. The convergence with respect to the cluster size will also be addressed. [1] A. Georges *et al.*, Rev. Mod. Phys. **68**, 14 (2006). [2] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).

O 58.80 Wed 18:15 Poster B1

Thermal transport in Graphite and related materials from general third order density functional perturbation theory. — •Lorenzo Paulatto, Michele Lazzeri, Francesco Mauri, and Giorgia Fugallo — IMPMC - UPMC/CNRS, Paris, France

We use a novel generic implementation of the third order anharmonic density-functional perturbation theory to study the phonon-phonon interaction in monolayer and bilayer graphene and in bulk graphite. We describe the anharmonic effects in terms of widening of the phonon linewidth and as a phonon mean free path in the medium. We discuss the temperature and q-point dependency of the linewidth.

We estimate the phonon-driven thermal transport in the single-mode relaxation time approximation, for room temperature and higher, and compare it to graphene and pyrolytic graphite experiments.

O 58.81 Wed 18:15 Poster B1

Electrochromic coatings based on an electron-conducting vapour-deposited organic semiconductor — •Juliane Weissbecker and Derck Schlettwein — Institute of Applied Physics, Justus Liebig University of Giessen, Heinrich Buff-Ring 16, 35392 Giessen, Germany

Thin films of phthalocyanine molecules are interesting for applications as electrochromic layers because of their strong light absorption and the strong change of colour upon oxidation or reduction. Because of instable cycling during oxidation, molecules are sought that are easily reduced (high electron affinity). The redox behaviour of vapour-deposited thin films (50 nm) of F_{16}PcCu was studied using simultaneous cyclic voltammetry and UV/Vis-spectroscopy. Upon electrochromic charging of the films electroneutrality has to be preserved by intercalating ions. The measurements were performed in contact to different electrolyte solutions and the influence of K^+, Na^+ or Li^+ ions is discussed. During an initial conditioning cycle a decrease of the cristallinity of the thin films was found and correlated with the ion diameter. An influence of ion diffusion on the overall current was not found. Almost constant potentials independent of the electrolyte were seen for the first reduction but differences were observed in subsequent waves. These differences are again correlated to the ion diameter and, hence, the interaction potential with the reduced molecules in the films.

O 58.82 Wed 18:15 Poster B1

Impedance Spectroscopy performed to measure and modify the oxide thickness on aluminum wires in an aqueous solution — •Felix Fiehler and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Metal wires are of interest as electrode materials in different applications also, e.g., in solar cells like dye-sensitized solar cells (DSC). Electron back transfer from the metal collector electrode to the iodine electrolyte or, even worse, corrosion of the metal can be a major problem. Some metals (including aluminum) are covered with a thin oxide layer, which is formed in contact with air providing a thin tunneling barrier, protecting the electrode from further corrosion by the electrolyte. This oxide layer, however, also can present a barrier in the electrodeposition of an active semiconductor and, in the DSC, an injection barrier for charge injection from the semiconductor to the metal. The thickness of the oxide therefore has to be controlled in detail for a successful application of aluminum wires in DSC. It is well known that electrochemical impedance spectroscopy (EIS) offers such a possibility to determine the thickness of the passivating oxide layer in situ during different applied potentials. The latter are of interest since the oxide thickness can be tuned by applying different positive or negative potentials relative to the standard electrode potential. Impedance spectra were measured for planar sheets and for wires of aluminum under variation of the applied DC potentials. The experimental results in the different potential ranges were discussed by use of established equivalent circuits.

O 58.83 Wed 18:15 Poster B1

III-V semiconductors for photoelectrolysis and their interface to the electrolyte — •Matthias M. May[1,2], Wolf-Dietrich Zabka[1,2], Oliver Supplie[1,2], Helena Stange[1,2], Christian Höhn[1], Hans-Joachim Lewerenz[1,3], and Thomas Hannappel[1,4,5] — [1]Helmholtz-Zentrum Berlin, Institute of Solar Fuels — [2]Humboldt-Universität zu Berlin, Institut für Physik — [3]California Institute of Technology, Pasadena, USA — [4]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik — [5]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

III-V semiconductors such as the dilute nitride GaP(N) represent an interesting material class for photoelectrolysis, especially in multi-junction approaches [1]. Corrosion and the charge-transfer efficiency towards the electrolyte [2] are challenges that have to be addressed by growth and/or electrochemical processing of the semiconductor surfaces. We prepare GaP(N) by metalorganic vapour phase epitaxy under in situ control with reflection anisotropy spectroscopy (RAS). Applying RAS and photoelectron spectroscopy at the semiconductor-liquid interface, we aim to improve the microscopic insight into the interface and to achieve in situ control of electrochemical processing. To this end, we perform H_2O adsorption in UHV as model-experiments, which we compare with results for the electrochemical environment.
[1] Döscher et al.,*ChemPhysChem* **13**:2899 (2012). [2] Kaiser et al, *ChemPhysChem* **13**:3053 (2012).

O 58.84 Wed 18:15 Poster B1

Scanning tunneling microscopy (STM) studies on the self-assembly of a twin monomer at the liquid-solid interface controlled by sonication time. A first step to the study of twin polymerization — Nguyen Doan Chau Yen[1], •Nguyen Thi Ngoc Ha[1], Patrick Kempe[2], Stefan Spange[2], and Michael Hietschold[1] — [1]Institute of Physics, Solid Surfaces Analysis Group, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Institute of Chemistry, Polymer Chemistry Group, Chemnitz University of Technology, D-09111 Chemnitz, Germany

Twin polymerization has been used as an elegant method for synthesizing nanostructured hybrid materials.Twin polymerization is a polymerization process which creates two different polymers out of a so-called twin monomer.The polymerization of a monomer 2,2*-spirobi[4H-132-

benzodioxasiline](SBS)is initiated by cleavage of the Si-O-C bonds. Here self-assembly of this SBS at the undecanol/HOPG interface is investigated by STM. It reveals a co-adsorption of SBS and undecanol solvent molecules in a regular pattern at ambient conditions. The nonplanar twin monomer can be clearly identified in the linear pattern with undecanol molecules oriented with their zig-zag plane orthogonally to the HOPG surface. Sonication has been proven to be a simple and powerful method to control the polymorphism of molecular adsorbates out of a solution.It is demonstrated that by sonicating SBS/undecanol solutions with different sonication time the co-adsorption of SBS and undecanol on HOPG can be controlled.

O 58.85 Wed 18:15 Poster B1

Influence of electrochemical adsorption on the conductive properties of thin platinum films in sulfuric acid — •Damian Bürstel and Detlef Diesing — Universität Duisburg - Essen, Fakultät für Chemie, Universitätsstrasse 2, D - 45141 Essen, Germany

The electrochemical hydrogen and oxygen reactions on platinum surfaces in acidic solution are still of great interest for electrocatalytic as well as for energy conversion research. In modern applications platinum is used in form of a few tens of nanometer thick metal films or as nanoparticles. At these dimensions one must be aware of the conductive properties of the metal film and particle and the influence of the changing metal–electrolyte interface on these properties during the electrochemical reactions.

The conductance of a thin platinum film on glass was measured by DC methods as well as AC methods at different frequencies simultaneously to cyclovoltammetric experiments in 0.5 M sulfuric acid. For the oxidation region the film conductance is mainly affected by the volumetric oxidation and reduction of the film and less effected by the metal–liquid interface properties. At hydrogen free platinum surfaces in the oxidation as well as in the electrochemical double-layer region a considerably high phase shift of the conductance with respect to the driving voltage across the film exists in AC measurements. In the course of hydrogen adsorption at $E_{HESS} < 0.4\,V$ a conduction parallel to the metal–liquid interface sets in with a low phase shift.

O 58.86 Wed 18:15 Poster B1

Investigation of spin-polarized transmission for electrons through Co/diamond/Co junctions — •Felix Huerkamp, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, Germany

We investigate the transmission properties of spin-polarized electrons at the interfaces of the metal-semiconductor hybrid system cobalt/diamond/cobalt within density-functional theory employing the generalized gradient approximation. The considered open system consists of three parts: the left and right semi-infinite cobalt leads, as well as the scattering region build by N layers of carbon atoms in a diamond structure. We use a Greens function technique which is based on the representation of the wave functions by Gaussian orbitals. This enables us to treat the scattering problem as a localized perturbation of a Co crystal. We have investigated junctions of hexagonal Co with C layers grown in (111) direction, as well as junctions of fcc Co with C layers oriented in (001) direction. We have identified different mechanisms, such as transmission resonances and overlapping interface states, that cause for specific energies and wave vectors a high transmission through the diamond layers. On the other hand, we find a vanishing transmission for energies within the Co bands and the diamond band gap at particular wave vectors even for thin C barriers. The results are discussed in dependence on the spin-direction and the number of carbon interlayers for hcp, as well as fcc Co leads.

O 58.87 Wed 18:15 Poster B1

Pulsed spray evaporation CVD of metal thin films: Role of reactor and precursor conditions — •Fedor Strigunov, Volkmar Zielasek, and Marcus Bäumer — Universität Bremen, Institut für Angewandte und Physikalische Chemie, Leobener Str. NW2, 28359 Bremen, Deutschland

A widely employed method to deposit thin films of metals and their compounds is chemical vapor deposition (CVD). A recently developed hydrogen-free approach to metal-CVD uses pulsed spray evaporation (PSE) delivery of simple and commercially available non-toxic metal-organic precursors dissolved in alcohols [1] and ease of use.

We have designed a compact PSE-CVD reactor that is attached to a UHV system for direct transfer to thin film analysis techniques such as XPS, STM, LEED or IR spectroscopy. We will present demonstrate the growth of thin Ni films on various substrates, including silicon oxide, without incubation time and without the need for any metallic seed layer. The efficiency of growth process and the quality of the resulting film strongly depend on several deposition parameters such as concentration of the precursors, deposition pressure, carrier gas flow rate, substrate temperature, deposition duration, spray pulse frequency and pulse width which have to be optimized for each new material and selected precursor. Besides the substrate temperature we have identified the concentration of water in the alcohol-carrier of precursor as very critical for the growth rate and deposition mechanism.

[1] P. A. Premkumar et al., Chem. Vap. Deposition, 13 (2007) 219

O 59: Invited Talk (Jörg Behler)

Time: Thursday 9:30–10:15 Location: H36

Invited Talk O 59.1 Thu 9:30 H36

Interatomic Potentials for Molecules, Solids, and Surfaces Based on Artificial Neural Networks — •Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

The reliability of the results obtained in molecular dynamics simulations strongly depends on the quality of the employed interatomic potentials. While electronic structure methods like density-functional theory provide an accurate description of many systems, the high computational costs limit the system size that can be studied. The construction of more efficient but equally reliable and unbiased interatomic potentials applicable to molecules, solids and surfaces is a frustrating challenge because of the very different types of bonding present for instance in organic molecules, ionic solids and metals. A wide range of functional forms has been suggested for a variety of systems, but a general-purpose potential suitable for all types of applications is still lacking. In recent years artificial neural networks (NNs) have become a promising new approach to fill this gap and to construct potential-energy surfaces with nearly ab initio quality for many systems. NN potentials are numerically very accurate, can be combined with any electronic structure method and, once constructed, allow to perform large-scale molecular dynamics simulations. Recent methodical developments aiming at applications to chemical processes at surfaces will be presented. The scope and current limitations of NN potentials will be discussed employing a number of realistic benchmark systems.

O 60: Focussed Session: Organic Materials for Spintronics: From Spinterface to Devices (jointly with DS, HL, and MA)

Since the first report of an organic spin valve in 2004, novel devices such as spin-OLEDs (organic light emitting diodes) and spin-OFETs (organic field effect transistors) as well as sensors based on magnetic resonance were developed. This rapid development of the field of organic spintronics is driven by the large spin life time in organic molecules, combined with the large diversity and flexibility of molecular synthesis and technological processing. Despite the tremendous progress, there are still many challenges which must be tackled. On one hand, it is desirable to achieve a computer-aided design for novel molecules that can keep their properties at the interfaces with the spin-injecting electrodes. On the other hand, novel technologies for the fabrication of spin devices and the spin transport properties of various molecules are being tested. Last but not least, the spin injection at spinterfaces, i.e. at the interface between the organic molecules and the ferromagnetic electrodes, is a key factor that still needs to be understood and controlled. This topical session aims to give an overview of the latest developments in the dynamic field of organic spintronics. (Organizers: Martin Aeschlimann, Uni Kaiserslautern; Bernd Büchner, IFW Dresden; Dietrich R. T. Zahn, TU Chemnitz)

Time: Thursday 9:30–13:30 Location: H32

Invited Talk O 60.1 Thu 9:30 H32

Organic Magnetoresistance: The effect of excitons on charge transport in organic semiconductors — •William Gillin — Queen Mary, University of London, UK

It has been known since 2003 that applying a magnetic field to an organic light emitting diode (OLED) will cause changes in both the light output (efficiency) of a device and the current through the device (organic magnetoresistance or OMR). The observation of this phenomenon has spurred a number of models to explain the observations but these can be classified in to two broad classes: excitonic and bipolaron. As the effect of the magnetic field is to apply a small perturbation to existing spin dependent processes that are affecting charge transport and recombination, the study of OMR provides an interesting new tool for understanding these processes. In this talk I will highlight the recent developments in the study of organic magnetoresistance and illustrate that the effect probably has several components which are all acting in parallel and which can have different signs and magnetic field dependencies. By developing an understanding of the different magnetic field characteristics of different processes we may open a door on to a new way of studying the interactions responsible for the fundamental operation of organic electronic devices.

Topical Talk O 60.2 Thu 10:00 H32

Metal-phthalocyanines: Materials for molecular spintronics — •Jens Kortus[1], Rico Friedrich[1], Torsten Hahn[1], Claudia Loose[1], and Martin Knupfer[2] — [1]TU Bergakademie Freiberg, Germany — [2]IFW Dresden, Germany

Metal-phthalocyanines (MPc) are very stable and can have different spin states depending on the transition metal ion. In this contribution we will discuss electronic, (magneto)optical and transport properties of MPc in view of possible application in spintronic devices.

In particular a recently investigated layered system of MnPc and F_{16}CoPc shows charge transfer at an interface between two metal phthalocyanines, which is investigated in detail using density functional theory. These results are of importance for the application of such interfaces in organic electronic devices because charge transfer considerably affects the energy level alignment and the transport behaviour of the respective hetero-junction. Since the transfer of charge is also connected to a transfer of spin and the hybrid system has a net spin of $S = 2$, such compounds could also be termed *spin-transfer materials* with future applications in the area of spintronics [1].

[1] S. Lindner, M. Knupfer, R. Friedrich, T. Hahn, J. Kortus Phys. Rev. Lett. 109 (2012) 027601-1/5

Topical Talk O 60.3 Thu 10:30 H32

Magneto-optical Kerr Effect Spectroscopy of Selected Phthalocyanines and Porphyrines — •Georgeta Salvan[1], Peter Robaschick[1], Frank Lungwitz[1], Michael Fronk[1], Carola Mende[1], Heinrich Lang[1], Rico Friedrich[2], Jens Kortus[2], and Dietrich R.T. Zahn[1] — [1]TU Chemnitz, 09126 Chemnitz, Germany — [2]2TU Bergakademie Freiberg, Freiberg 09596, Germany

Phthalocyanines and porphyrines find nowadays many applications from pigments to organic electronics. Nevertheless, they still have a special charm for fundamental investigations thanks to the large flexibility of their molecular structure. This work focuses on the influence of the molecular spin ground state on the room temperature magneto-optical activity of some phthalocyanines and porphyrins. The films in the typical thickness range between 30 nm and 100 nm were prepared by organic molecular beam deposition in high vacuum. Magneto-optical Kerr effect (MOKE), which is commonly used to study the magnetic properties of inorganic ferromagnetic layers or magnetic nanostructures, is measured here spectroscopically in the region of the Q and B absorption bands of phthalocyanines and porphyrines. From this the magneto-optical Voigt constant is calculated numerically and can be correlated to the electronic properties of the molecules. For instance, the hybridisation of Co3d states with the HOMO π-orbital of CoPc leads to additional features in the magneto-optical spectra compared to e.g. CuPc. The magnitude of the Voigt constant in the Q band is hardly sensitive to the molecular spin, but highly sensitive to the orientation of the molecules with respect to the substrate plane.

Topical Talk O 60.4 Thu 11:00 H32

Molecular Quantum Spintronics — •Mario Ruben — Institut für Nanotechnologie (INT), Karlsruhe Institut für Technologie (KIT) — Institut de Physique et Chimie (IPCMS); Université de Strasbourg (UdS)

Molecules can be considered as physical Quantum Objects. Magnetic molecules consist of an atomic core of one-to-few open spin ions surrounded by a shell of organic material. At low temperature such molecular spin objects behave as simple, few-level systems.[1,2] Since quantum coherence and stable entanglement of electron spins are extremely difficult to achieve, alternative concepts propose the use of nuclear spins as quantum information carrier. Nuclear spins are extremely well isolated from environment and less prone to decoherence, and the coherent manipulation can be adapted by tailoring the molecular environment. However, although being well isolated from their surroundings, nuclear spins have to be addressed, ideally electronically since complementary with existing technologies. The delicate balance between decoupling of the magnetic molecule for stable coherence and connecting it for read out can be carried out by synthetic engineering of the molecular components. The first example of a completely electronic read out of a nuclear spin of a lanthanide ion (bearing electron and nuclear spins) embedded in a magnetic molecule TbPc2, was recently reported.[3] [1] M. Urdampilleta et.al. Nature Mater. 10, 502 (2011) [2] J. Schwöbel, et. al. Nature Comms. 2, 1953 (2012) [3] R. Vincent, et. al. Nature 488, 357 (2012)

Coffee break (15 min)

Topical Talk O 60.5 Thu 11:45 H32

Nanomembrane based electrodes for contacting ultra-thin organic layers — •Carlos Cesar Bof Bufon[1], Celine Vervacke[2], Maria Esperança Navarro Fuente[2], Dominic J. Thurmer[2], Christian Müller[5], Michael Fronk[3], Georgeta Salvan[3], Dietrich R. T. Zahn[3], and Oliver G. Schmidt[2,4] — [1]Brazilian Nanotechnology National Laboratory, CNPEM, PO Box 619, 13083-970, Campinas, Brazil — [2]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, 01069, Dresden, Germany — [3]Semiconductor Physics, Chemnitz University of Technology, Reichenhainerstrasse 70, 09107, Chemnitz, Germany — [4]Material Systems for Nanoelectronics, Chemnitz University of Technology, Reichenhainerstrasse 70, 09107 Chemnitz, Germany — [5]Physics Departament, UFPR, Curitiba, Brazil

One of the main challenges for accessing the electronic properties of ultrathin organic layers (UOL), and consequently their application for future devices, consists of connecting such layers to the external word. Two main problems usually arise by trying to vertically connect UOLs: i) the interdiffusion of metallic atoms into the sub-10nm molecular layers, which leads to the damaging and/or the modification of the final device behavior; ii) the presence of pin-holes across the molecular layer, which is responsible for short circuited junctions. Here we discuss the fundamentals, potentialities and limitations of using rolled up nanomembranes as top electrodes for contacting a variety of UOLs, including self-assembled monolayer's and ultra-thin organic semiconducting layers.

Topical Talk O 60.6 Thu 12:15 H32

Spinterfaces as microscopic spin traps — •Mirko Cinchetti — Department of Physics and Research Center OPTIMAS, University of

Kaiserslautern, Kaiserslautern, Germany

Interfaces between ferromagnetic materials and organic semiconductors - also known as spinterfaces - constitute an incredibly rich playground in the field of spintronics. For example, spinterfaces have the potential to be implemented as tunable spin filters, which will pave the way to a whole new class of advanced, i.e., actively controlled spintronics devices. The progress in the field of spinterface science depends thus critically on elucidating the still unexplored spin-dependent carrier dynamics at such hybrid interfaces.

We use time-resolved two-photon photoemission to optically pump and probe a hybrid electronic state forming at the prototypical spinterface between cobalt and the organometallic complex tris(8-hydroxyquinolinato)aluminium (Alq3). We generate a transient spin polarization in the hybrid interface state, and follow its behavior in four dimensions: energy, time, spin and momentum. We find that electrons are confined at the Co-Alq3 interface for times in the range of 0.5-1 ps, and that the confining potential is strongly spin dependent. Such spin-dependent trapping behavior elucidates the fundamental microscopic origin of the spin-filtering properties at spinterfaces, which is important for the design of next-generation spintronics devices based on tunable organic spin filters.

O 60.7 Thu 12:45 H32

ESR study of the magnetic properties of the MnPc − F_{16}CoPc dimer — •Azar Aliabadi, Susi Linder, Martin Knupfer, Yulia Krupskaya, Vladislav Kataev, and Bernd Büchner — IFW Dresden, 01069 Dresden

Photoemission spectroscopy has demonstrated a charge transfer at the interface between two transition metal phtalocyanines (MnPc and F_{16}CoPc) indicating the formation of a MnPc$^{\delta+}$/F_{16}CoPc$^{\delta-}$ heterojunction [1]. In this work, the MnPc-F_{16}CoPc dimer system with charge transfer was investigated using ESR spectroscopy at different temperatures. Comparison between ESR spectra of the parent compounds (MnPc and F_{16}CoPc powders) and of the product of the reaction (MnPc/F_{16}CoPc mixed powder) has revealed characteristic features due to the formation of the MnPc − F_{16}CoPc dimer. We discuss distinct magnetic properties of the MnPc − F_{16}CoPc dimer and their possible relation to the charge transfer in the studied complex.

[1] S. Lindner, M. Knupfer, R. Friedrich, T. Hahn, and J. Kortus, *Phys. Rev. Lett.* **109**, 027601 (2012).

O 60.8 Thu 13:00 H32

Influence of surface interaction on the properties of single-molecule-magnets — •David Klar[1], Andrea Candini[2], Bernhard Krumme[1], Loic Joly[3], Svetlana Klyatskaya[4], Jean-Paul Kappler[3], Mario Ruben[3,4], and Heiko Wende[1] — [1]Fakultät für Physik und CENIDE, Universität Duisburg-Essen — [2]Centro S3 Modena, Istituto Nanoscienze - CNR — [3]Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg — [4]Institute of Nanotechnology, Karlsruhe Institute of Technology

Due to the consecutive downsizing of devices, single-molecule-magnets as building blocks for spintronic applications are of high interest for actual research. The remanent behavior, caused by the single-ion anisotropy, of $TbPc_2$ molecules in bulk samples at less than 5 K is reported in the literature. Our goal is to investigate and to understand the influence of the surface on the properties of the $TbPc_2$ molecules deposited onto a substrate. Therefore we study submonolayer coverages of $TbPc_2$ molecules on ferromagnetic surfaces like Ni, and on a very inert surface of highly oriented pyrolytic graphite (HOPG) that should maintain the properties of isolated molecules. By XAS and XMCD we analyze the element specific magnetic and electronic properties. The low interaction with the HOPG surface hardly affects the magnetic properties of the molecules and we were able to observe a remanent magnetization, but only at very low temperatures ($T < 4$ K). On the Ni surface an indirect exchange leads to an antiferromagnetic coupling between the molecules and the surface. As a result, we obtained a remanent magnetization at higher temperatures ($T \approx 100$ K).

O 60.9 Thu 13:15 H32

Paramagnetic organic radicals on rutile TiO2(110) single crystals — •Reza Kakavandi, Sabine-Antonia Savu, Thomas Chassé, and Maria Benedetta Casu — Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany

A novel class of organic compounds, namely the nitronyl nitroxide radicals, has recently gained attention because of its magnetic property. In this work a pyrene-substituted nitronyl nitroxide radical (NitPyn) deposited on well characterized rutile TiO2(110) single crystals has been investigated by using X-ray photoemission spectroscopy (XPS) and near edge X-ray absorption fine structure spectroscopy. The mechanism of molecular adsorption on the well defined surface, the chemical environment at the interface and the electronic structure of thin films are discussed by analyzing the XPS core level signals. The persistence of the paramagnetic character of the molecules is also discussed with respect to the chemisorption on the surface. Our studies clarifies the orientation of the molecule in the thin films as a function of film thickness as well as the influence of the substrate, identifying the fine balance between molecule-molecule and molecule-substrate interactions.

O 61: Organic Electronics and Photovoltaics I (jointly with CPP, DS, and HL)

Time: Thursday 9:30–13:00 Location: H34

Invited Talk O 61.1 Thu 9:30 H34

Influence of morphology on organic solar cell performance comparing crystalline diindenoperylene (DIP) and its amorphous derivative tetraphenyldibenzoperiflanthene (DBP) — Stefan Grob, Mark Gruber, Ulrich Hörmann, and •Wolfgang Brütting — Institute of Physics, University of Augsburg, Germany

The DIP molecule, consisting of seven benzene and two cyclopentadiene rings, forms the backbone of the DBP molecule, which has two further benzene rings and four additional, rotatable phenyl groups. Compared to the planar arrangement of DIP, the four phenyl groups give DBP a more three-dimensional shape, changing the growth behavior in thin films completely. While we observe crystalline domains of almost upright standing DIP, layers of DBP exhibit an amorphous character and therefore a relatively small exciton diffusion length, being about ten times shorter than that of its crystalline counterpart. However, the drawback of the upright standing arrangement of DIP molecules is the unfavorable orientation of the transition dipole moment resulting in a low absorption coefficient. In contrast, the structural disorder in DBP combined with a little smaller optical gap leads to light absorption which is about eight times higher than in DIP, whereby the short-circuit current density almost doubles in corresponding solar cell devices. Moreover, open circuit voltages are high and - due to similar energy level alignments - comparable, by using the materials both as donor with C60 (0.9 V) and as acceptor with 6T (1.2 V). Based on these results, we discuss the influence of different film structure and morphology on electrical transport and device performance.

O 61.2 Thu 10:00 H34

Influence of fluorine content in manipulating the nanomorphology of PTB7:PC70BM bulk heterojunction systems — •Shuai Guo[1], Jing Ning[1], Volker Körstgens[1], Yuan Yao[1], Chen Lin[1], Stephan Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany

Polymer-based photovoltaics have drawn tremendous attention in both basic research and application fields during the last decade. Here, the up-to-date highest efficient bulk heterojunction system PTB7 with varied fluorine content and the fullerene derivative PC70BM are thoroughly investigated. It is known that the amount of fluorine along the polymer chain strongly influences the film formation and therefore the solar cell performance. Additionally, it is of great interest to explore the effect of solvent additive 1,8-diiodooctane (DIO) on differently fluorinated films. To address the relation between the morphology and efficiency completely, a series of measurements have been done. The film surface structure is investigated by optical microscopy and AFM. The inner film structures, crystal orientation as well as the crystallinity are probed by advanced scattering techniques such as XRR, GISAXS and GIWAXS. By integrating all data, the three-dimensional morphology of the active layer is detected. Consequently, the different morphologies introduced by varying the fluorine content and the addition of DIO are determined and compared with the corresponding performance of these systems.

O 61.3 Thu 10:15 H34

Influence of nanostructural changes on the charge carrier dynamics in PTB7 based solar cells — •Andreas Zusan[1], Andreas Baumann[2], Jens Lorrmann[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

For organic bulk heterojunction solar cells, the blend morphology is one of the most crucial parameters influencing the device performance. Inducing nanostructural changes by means of the use of processing additives is a common practice to increase the power conversion efficiency. Hence, understanding the effect of modified structural properties of organic layers on the charge carrier transport and lifetime is a key issue for further progress in organic photovoltaics. In this context, we applied our novel charge extraction technique OTRACE (Open Circuit Corrected Transient Charge Extraction) to high efficiency solar cells made from the low-bandgap polymer PTB7 in combination with $PC_{70}BM$ using the solvent additive diiodooctane (DIO). The results show two different nongeminate decay regimes identified as a fast direct recombination of free polarons and a trap assisted decay. We find that the DIO induced alteration of the morphology significantly reduces the recombination order of the first regime, whereas it has no influence on the second part arising from the delayed emission of trapped charges. Our explanation based on a multiple-trapping-and-release approach clarifies the large impact of phase separation on charge carrier dynamics.

O 61.4 Thu 10:30 H34

Diffusion limited charge generation from fullerene excitons in low bandgap polymer solar cells — •Clare Dyer-Smith, Ian Howard, and Frédéric Laquai — Max Planck Institut für Polymerforschung, Mainz, Germany

Organic solar cells with high power conversion efficiencies have been realised in recent years by the use of low bandgap polymers in combination with C70-based electron acceptors to provide good absorption coverage across the entire solar emission spectrum. Diffusion-limited charge generation from fullerene excitons has been observed in such blends, including the high-performance PTB7:PC70BM blend system which is the subject of the present study. We characterise the diffusion-limited charge generation from fullerene excitons in this system using transient absorption and photoluminescence spectroscopy. Fitting to a simple exciton quenching model allows us to determine the size of fullerene domains in the blend, showing quantitatively how blend morphology limits device performance, and allowing us to identify selection criteria for the optimum blend morphology in devices based upon light-absorbing fullerene acceptors.

O 61.5 Thu 10:45 H34

Impact of molecular weight on the intrinsic charge carrier mobility of Si-PCPDTBT:[C70]PCBM thin films — •Andreas Fritze[1], Andreas Sperlich[1], Andreas Zusan[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

We investigated the influence of the molecular weight on the performance of solar cells from solution processed Si-PCPDTBT:[C70]PCBM blends. A significant increase in the short circuit current density j_{SC} was found with increasing molecular weight of the polymer. To explain this behavior, we performed transient microwave conductivity (TRMC) experiments and found much higher intrinsic mobilities in thin films based on the higher molecular weight donor. In order to distinguish between the influence of intra- and intermolecular charge transport on the obtained intrinsic TRMC mobility, we used two different solvents to influence the molecular environment in the film. We discuss our findings in view of the impact of the local order, influenced by the molecular weight on the performance of organic solar cells.

O 61.6 Thu 11:00 H34

Charge generation and recombination in PCPDTBT:PCBM and PSBTBT:PCBM bulk heterojunction photovoltaic blends — •Fabian Etzold, Ian Howard, Michael Meister, and Frédéric Laquai — Max Planck Research Group for Organic Optoelectronics, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We present a comparative study of the photophysical processes leading to photocurrent generation and photocurrent loss in photovoltaic blends of the low-bandgap polymer PCPDTBT with PCBM and its silicon-substituted analogue PSBTBT with PCBM studied by Vis-NIR transient absorption pump-probe spectroscopy and variable time-delay double-pump photocurrent extraction experiments. Our experiments demonstrate that the power conversion efficiency of PCPDTBT:PCBM blends is largely limited by sub-nanosecond geminate recombination of interfacial charge-transfer states plus fast non-geminate recombination of free charges competing efficiently with charge extraction. In comparison photovoltaic blends of the silicon-substituted polymer PSBTBT with PCBM exhibit significantly less geminate recombination in conjunction with much slower non-geminate recombination of free charges leading in turn to substantially higher photocurrents and fill factors and thus overall increased photovoltaic performance. We also observed a pronounced excitation wavelength dependence of the photophysical processes occurring after excitation of either the polymer or the fullerene component of the blend at different photon energies. [1] F. Etzold et al., J. Am. Chem. Soc. 2012, 134 (25), 10569-10583.

15 min. break

O 61.7 Thu 11:30 H34

Charge Generation in PBDTTPD:PCBM and Si-PCPDTBT:PCBM Solar Cells: The Influence of Excess Photon Energy and Electronic Energy Level Offsets — •Steve Albrecht[1], Koen Vandewal[2], Alberto Salleo[2], and Dieter Neher[1] — [1]University of Potsdam, Soft Matter Physics, Potsdam, Germany — [2]Stanford University, Department of Materials Science and Engineering, Stanford, USA

In the last years a dramatic increase in organic solar cell efficiency has been reported with polymers and fullerene derivatives processed from solution. However, the fundamental process involved in the conversion of absorbed photons to free charges is still not fully understood. In this work, we use time delayed collection field (TDCF) **[1]** with variable excitation wavelength to gain inside into the effect of the excess photon energy on the quantum efficiency and field-dependence of free charge carrier generation. With two high efficiency model systems showing either field independent CT-state splitting (PBDTTPD:PCBM) or a weak field-dependence of free charge formation (Si-PCPDTBT:PCBM), we show how the field-dependence changes with direct CT state excitation in the absorption region below the band-gap. Additionally, we show how generation and bimolecular recombination is affected when the fullerene derivative PCBM is exchanged by higher LUMO adducts ICMA, ICBA or ICTA with reduced driving force for CT-state splitting.

[1] Albrecht, S.; Janietz, S.; Schindler, W.; Frisch J.; Neher D., Journal of the American Chemical Society 134 (36), 14932 (2012).

O 61.8 Thu 11:45 H34

Sub-Bandgap Absorption in Polythiophene–Fullerene Heterojunctions: Experiment and Theory — •Wichard Beenken, Felix Herrmann, Martin Presselt, Harald Hoppe, Sviatoslav Shokhovets, Gerhard Gobsch, and Erich Runge — Technische Universität Ilmenau, Institut für Physik and Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany

Most high-performance organic solar cells base on P3HT/PCBM bulk-heterojunctions. Spectroscopy of the sub-bandgap region, i.e., below the bulk absorption of the individual components, provides unique opportunities to study interface-related properties. In order to characterize some of the unsettled spectral features, we applied quantum-chemical calculations of a oligothiophene–fullerene model complex, which in particular allow us to identify spectral signatures of charge-transfer excitons in the sub-bandgap absorption and external quantum efficiency.

O 61.9 Thu 12:00 H34

A new multiscale modeling method for simulating the loss processes in polymer solar cell nanodevices — •Anton Pershin, Sergii Donets, and Stephan A. Baeurle — Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany

The photoelectric power conversion efficiency of polymer solar cells is till now, compared to conventional inorganic solar cells, relatively low with maximum values ranging from 7% to 8%. This essentially relates to the existence of exciton and charge carrier loss phenomena, significantly reducing the performance of polymer solar cells. Here, we introduce a new computer simulation technique [1], which permits to explore the causes for the occurrence of such phenomena at the nanoscale and to design new photovoltaic materials with optimized opto-electronic properties. Using our approach, we find that the disjunction of continuous percolation paths leads to the creation of dead ends, resulting in charge carrier losses through charge recombination. Moreover, we observe that defects are characterized by a low exciton dissociation efficiency due to a high charge accumulation, counteracting the charge generation process. Finally, by analyzing the photovoltaic behavior of the nanostructures under different circuit conditions, we demonstrate that charge injection at the electrodes determines the impact of the defects on the solar cell performance. [1] A. Pershin, S. Donets, S.A. Baeurle, J. Chem. Phys. 136, 194102 (2012).

O 61.10 Thu 12:15 H34

Morphology and Charge Transport in Polythiophene/PCBM Blends: Insight from Molecular Simulations — •Olga Guskova[1], Julia Romanova[2], Andreas John[1], Peter Friedel[1], and Jens-Uwe Sommer[1,3] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]University of Namur, Namur, Belgium — [3]TU Dresden, Dresden, Germany

Combined structural-computational approach to study the organic photovoltaic materials, namely mixtures of polythiophenes (donor, D) and [6,6]phenyl-C61-butyric acid methyl ester (acceptor, A) was applied. The quantum mechanical computational level was used (1) to improve the force field for subsequent molecular dynamics (MD) modeling, (2) to calculate the ionization energies, electron affinities, HOMO/LUMO energies and charge transfer characteristics of D/A pair. We have performed a large-scale all-atomistic MD simulation to investigate both the geometry of D/A interface between two crystals and the D/A blend morphology in self-organized systems (the ordering and molecular orientation, the formation of polythiophene paracrystalls and PCBM-rich phases in amorphous regions of polythiophene).

O 61.11 Thu 12:30 H34

Electroabsorption spectroscopy on organic pin solar cells — •Ellen Siebert-Henze, Vadim G. Lyssenko, Janine Fischer, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, George-Bähr-Str. 1, Dresden, Germany

The built-in voltage has a significant impact on the solar cell performance, but its origins are controversially discussed. In our work we determine the built-in voltage of small molecule organic solar cells based on the pin concept by electroabsorption spectroscopy (EA).

EA detects the change in absorption caused by an electrical field (Stark effect). A change in DC bias on the device results in a variation of the Stark signal. It is probed adding an AC voltage on top of the DC bias enabling the detection using a lock-in amplifier. Thus, the information about the built-in voltage can be evaluated.

As a model system, flat heterojunction solar cells containing C_{60} as acceptor and MeO-TPD as donor material are investigated. The doping concentration of both the hole and the electron transport layer is modified and it is shown that there is an influence of the consequential change of their work functions on the built-in voltage. Both the short-circuit current as well as the fill factor increase for larger built-in voltages.

O 61.12 Thu 12:45 H34

First-principles calculations of the TCO-Organic interface in an OLED — •Arno Fey[1], Paul Erhart[2], and Karsten Albe[1] — [1]Fachbereich Material- und Geowissenschaften, Technische Universität Darmstadt, Darmstadt, Germany — [2]Department of Applied Physics, Chalmers University of Technology, Gothenburg, Sweden

The ongoing development in the field of organic light emitting diode (OLED) technology and the continuously improvement towards higher efficiencies has created a need to understand the interaction between the different layers in an OLED. In this contribution we focus on the interface of the transparent conductive oxide (TCO) and the organic molecule. The interaction between the polar and hydrophilic oxide surface on the one side and the organic and non-polar thin film on the other side determines the growing of the organic film and therefore directly influences the conductivity. The calculations based on the density functional theory (DFT) were carried out using the Vienna ab initio simulation Package (VASP) with Generalized Gradient Approximations (GGA).

O 62: Focussed Session: Frontiers of Electronic Structure Theory VI (jointly with HL and TT)

Time: Thursday 10:30–13:15 Location: H36

Topical Talk O 62.1 Thu 10:30 H36

Atomic-scale design of energy materials — •Karsten W. Jacobsen — CAMD, DTU Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The design of new materials for more efficient production and use of sustainable and clean energy is of utmost importance for the standard of living all over the World the coming years. In the talk I shall describe some computational efforts to design new materials related to solar energy in particular to the conversion of light into hydrogen fuel through water splitting. We have employed computational screening to search for stable semiconductor materials with an appropriate bandgap, band edge alignment, and with sufficient stability to be relevant for light-induced water splitting. In particular we have focused on materials in the cubic perovskite structure but also more generally materials in the ICSD database. The screening of bandgaps is performed using the so-called GLLB-functional which is shown to give reasonable estimates of light absorption for a number of different systems. The stability of the materials towards dissolution in water is investigated through the construction of Pourbaix diagrams combining DFT calculations and experimental information about solution energies.

The talk will also cover some recent efforts in using machine-learning techniques to develop new electronic density functionals. The functional construction uses Tikhonov regularization to obtain smooth functionals and employs bootstrapping to avoid overfitting. The new functionals are named Bayesian Error Estimation Functionals (BEEF) because they automatically offer error estimation on calculated results.

O 62.2 Thu 11:00 H36

A new computational screening approach for co-catalysts for water splitting:
Disentangling electron and proton transfer. — •Harald Oberhofer, Daniel Berger, Ran Jia, and Karsten Reuter — TU München, Germany

Recently, computational screening techniques have made great progress in the identification and classification of promising new materials for (photo-)catalytic water splitting. Yet, contributions of so called co-catalysts—nano-sized particles enhancing the reaction kinetics—have so far not been addressed. In our contribution we present a novel first-principles thermodynamic approach based on earlier work by Nørskov and Rossmeisl [J. Phys. Chem. B **108**, 17886 (2004)] to gauge the efficiency of co-catalyst particles and search for favourable combinations of catalyst surface and co-catalyst particle. Additionally, we study reaction pathways other than the commonly assumed proton-coupled electron transfer. Our results show that these uncoupled paths can lead to new, unexpected behaviour: Catalysts predicted to have a good reactivity considering only coupled mechanisms might actually get stuck in charged intermediates, while others can be much more reactive than anticipated.

O 62.3 Thu 11:15 H36

An extended Pareto approach to computational materials design — •Kurt Lejaeghere[1], Stefaan Cottenier[1,2], and Veronique Van Speybroeck[2] — [1]Center for Molecular Modeling, Ghent University, Zwijnaarde, Belgium — [2]Department of Materials Science and Engineering, Ghent University, Zwijnaarde, Belgium

Because of competing design criteria, it is often hard to decide on one particular material as the best solution for a given need. A multidimensional optimization strategy can already narrow down the initial large set of candidates to a much smaller number of promising materials, the Pareto-optimal set. Quite often, however, this set contains more materials than can be afforded for further systematic examination. An ordering within this set, highlighting the most promising candidates, would be very useful to expedite the design process. Conventional Pareto approaches cannot offer such a ranking. We present an algorithm to do exactly this.

This procedure is applied to a set of binary tungsten alloys to look for a candidate first-wall material for nuclear fusion purposes. Because of the harsh operating conditions inside (future) fusion reactors, materials selection is a critical aspect there. Tungsten is a promising first-wall material, but several issues, such as room-temperature brittleness, are still to be resolved. Alloying tungsten with other elements is one possible way of overcoming these problems. By combining a computational screening study (at the DFT-PBE level) with our extended Pareto analysis, a select number of alloys is presented as most promising candidates for further experimental investigation.

O 62.4 Thu 11:30 H36

Automated system for massive sets of first-principles calculations — •Atsushi Togo and Isao Tanaka — Department of Materials Science and Engineering, Kyoto University, Yoshida-honmachi, Sakyo-ku, Kyoto, Japan

Large systematic sets of first principles calculations can provide information that cannot be obtained merely by a single calculation. Computation of phonon, cluster expansion, and data mining are typical examples that require massive sets of calculations. If each of single calculation is independent to the others, it is trivial to handle massive calculations consecutively. However it is annoying if a calculation has to wait for the previous calculations to finish. We have been developing an automated system. This system is composed of an automation algorithm and interfaces for a first-principles calculation code (VASP) and a batch-queuing system (grid engine). Small tools are prepared to handle crystal symmetry and dynamical properties. As an application, an algorithm for crystal structure search is implemented. The automation algorithm is as follows. We define 'task'. A task is made of 'task elements', where each task element is designed to be also a task. A task may be composed of a series of task elements. In this case, each task element waits for the previous task element to finish. A task may be composed of task elements that are mutually independent. In this case, all task elements are distributed into computers at the same time. By describing each kind of task in a similar manner, a task is easily built into the other task as a task element.

O 62.5 Thu 11:45 H36

Bandgap Engineering via Nanoporosity in ZnO — Ilker Demiroglu[1], Sergio Tosoni[1], Francesc Illas[1], and •Stefan Bromley[1,2] — [1]Departament de Química Física and Institut de Química Teòrica i Computacional, Universitat de Barcelona (IQTCUB), 08028 Barcelona, Spain — [2]Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, Spain

Following previous studies [1-3], we have mined databases of 4-connected nets to generate novel nanoporous ZnO structures. Using density functional theory and GW calculations, we calculate the energetic stability and band gaps of >80 distinct nanoporous ZnO solids. We find that the degree and type of nanoporosity is inextricably linked with band gap magnitude. Increasing the degree of nanoporosity tends reduce energetic stability and increase the band gap. Within this tendency, we also find significant variations in band gap (~0.5 eV) for structures with very similar densities or energetic stabilities but different types of nanoporosity (e.g. pore size). We estimate that altering the degree/type of nanoporosity could allow tailored band gap values up to ~4.2 eV. This proposed nanomorphological approach to band gap engineering potentially opens the door to optoelectronically tunable sensors, solar cells and other unforeseen devices which could take advantage of this versatile combination.

[1] J. Carrasco, F. Illas and S. T. Bromley, PRL 99, 235502 (2007). [2] M. A. Zwijnenburg, F. Illas and S. T. Bromley, PRL 104, 175503 (2010). [3] D. Stradi, F. Illas, S. T. Bromley, PRL 105, 045901 (2010).

O 62.6 Thu 12:00 H36

Phonon-mediated quantum processes in materials — •Emmanouil Kioupakis — University of Michigan, Ann Arbor, MI, USA

Higher-order quantum processes enabled by the coupling of charge carriers to lattice vibrations can play an important role in the operation of modern electronic and optoelectronic devices. First-principles calculations based on density functional theory can provide insight into the fundamental nature of phonon- assisted quantum processes in materials and their impact on device performance. In this talk, I will discuss our recent work on phonon-assisted quantum processes with first-principles techniques. I will show how phonon- assisted Auger recombination gives rise to the observed efficiency loss in nitride light-emitting diodes. Moreover, I will demonstrate that first-principles techniques can accurately reproduce the phonon-assisted optical absorption spectrum of silicon. Last, I will show that phonon-mediated free-carrier absorption leads to optical loss in transparent conducting oxides and semiconductor lasers. The developed techniques are general and can be applied to study phonon-assisted quantum processes in any material. This work was done in collaboration with C. G. Van de Walle, P. Rinke, K. Delaney, A. Schleife, F. Bechstedt, D. Steiauf, H. Peelaers, J. Noffsinger, S. G. Louie, and M. L. Cohen.

O 62.7 Thu 12:15 H36

Electron-hole puddles in the absence of charged impurities — •Marco Gibertini[1,2], Andrea Tomadin[2], Francisco Guinea[3], Mikhail I. Katsnelson[4], and Marco Polini[2] — [1]Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland — [2]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy — [3]Instituto de Ciencia de Materiales de Madrid (CSIC), Sor Juana Inés de la Cruz 3, E-28049 Madrid, Spain — [4]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands

It is widely believed that carrier-density inhomogeneities ("electron-hole puddles") in single-layer graphene on a substrate such as quartz are due to charged impurities located close to the graphene sheet. In this talk we demonstrate by using a Kohn-Sham-Dirac density-functional scheme that corrugations in a real sample are sufficient to determine electron-hole puddles on length scales that are larger than the spatial resolution of state-of-the-art scanning tunneling microscopy.

O 62.8 Thu 12:30 H36

Ab-initio transport calculations of functionalized graphene flakes — •Michael Walz, Alexei Bagrets, and Ferdinand Evers — Institut für Nanotechnologie, Karlsruher Institut für Technologie (KIT), D-76021 Karlsruhe, Germany

These days, nanoelectronics is focused on molecular systems such as single organic molecules, graphene ribbons, functionalized graphene flakes, carbon nanotubes.

In our project, we calculate the transmission and the local current density in graphene flakes which are functionalized by adsorbed atoms. We are especially interested in current patterns associated with the functionalized carbon atoms and the role of quantum interference effects.

Performing such calculations starting from first principles is challenging because of high computational costs. On this account, we work with the parallelized *ab-initio* framework FHI-aims, on top of which we implement our own transport calculations using non-equilibrium Green's functions (NEGF) techniques with standard functionals [1,2]. Such *ab-initio* transport studies already exist for the field of Molecular Electronics. Our effort presents a first step towards the broader scope of meso-sized molecular materials in general.

[1] V. Blum *et al.*, Comput. Phys. Commun. **180**, 2175 (2009).

[2] A. Arnold *et al.*, J. Chem. Phys. **126**, 174101 (2007).

O 62.9 Thu 12:45 H36

Thermionic emission from metal surfaces: A first principles study — •Johannes Voss[1], Sharon Chou[1], Aleksandra Vojvodic[1,2], Igor Bargatin[3], Roger Thomas Howe[1], and Frank Abild-Pedersen[2] — [1]Stanford University, USA — [2]SLAC National Accelerator Laboratory, USA — [3]University of Pennsylvania, USA

The ability to lower the temperatures required for sufficient electronic emission from hot cathodes would lead to more efficient thermionic energy converters and electron guns. Thermionic emission of electrons from metal surfaces is governed by the work function and tunneling probabilities. While the former can be extracted easily from ab initio band structure calculations, for the latter, scattering properties of the surface need to be taken into account.

Here, we present density functional theory calculations of thermionic emission currents based on a non-equilibrium Green's function approach. We compare these results to experiments both for clean and coated metal surfaces. Based on an analysis of interactions in the coating layers, we suggest design pathways for new materials with higher emission current densities.

O 62.10 Thu 13:00 H36

Comparative computational study of Li, Na, and Mg diffusion in bulk Si: influence of cooperative effects, vibrations, and

atom-centered bases — •Sergei Manzhos[1], Oleksandr Malyi[1], and Teck L. Tan[2] — [1]Department of Mechanical Engineering, National University of Singapore, Blk EA #07-08, 9 Engineering Drive 1, Singapore 117576 — [2]Institute of High Performance Computing, A*STAR, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632

Si is one of the most efficient anode materials for Li ion batteries. At the same time, for bulk storage and/or high energy density applications, Na and Mg are advantageous due to low cost and abundance of Na and high energy density in the case of Mg. Yet the performance of Si as anode material for Na and Mg batteries is still understudied. We present a comprehensive computational study of diffusion barriers of Li, Na, and Mg in Si including cooperative effects (influence of neighboring metal atoms on the barrier). Interactions between metal atoms in Si cause a significant lowering of the diffusion barrier; this effect is increasing when going from Li to Na to Mg. Zero-point vibrations (ZPE) affect migration barriers strongly and differently for different metals, increasing the barrier for Li diffusion, having little effect on Na, and decreasing the barrier for Mg. Most calculations to date for metal ion diffusion in battery electrodes were done using plane-wave based codes. We present an analysis of the effects due to atomic-centered basis selection. To the best of our knowledge, this is the first study of the effects of ZPE and atomic-centered bases on the computed properties of battery electrodes.

O 63: Plasmonics and Nanooptics V

Time: Thursday 10:30–13:00 Location: H38

O 63.1 Thu 10:30 H38

Photothermal control of light propagation — •André Heber and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, D - 04103 Leipzig

Photons are an ideal choice when it comes to telecommunication. They can transfer information at high bandwidth over large distances with low losses. Therefore it is desirable to directly manipulate these signals by other photons which is a difficult task as photon photon interactions are intrinsically weak. Different schemes have been proposed to make beams of light interacting with each other. Some of these include nonlinear optical effects, optical resonators and single quantum systems such as single molecules. Our approach relies on the absorption of a single gold nano-particle which is exposed to an optical signal. It dissipates the excitation energy into the environment as heat creating a temperature profile. This particle is embedded into a nematic liquid crystal which changes its state of matter from the birefringent nematic to the isotropic phase at ambient temperature. The polarisation change by the liquid crystal depends on the thickness of the nematic layer. Therefore the transmission of a second laser beam through the nematic layer in polarisation contrast depends on the intensity of the signal beam. We demonstrate a 100% intensity modulation.

O 63.2 Thu 10:45 H38

Arrays of plasmonic particles for optical trapping — •Manuel Gonçalves[1], Fabian Enderle[2], Alfred Plettl[2], Paul Ziemann[2], and Othmar Marti[1] — [1]Ulm University - Institute of Experimental Physics, Ulm, Germany — [2]Ulm University - Institute of Solid State Physics, Ulm, Germany

Optical trapping based on plasmonic structures has been employed to exert electromagnetic forces on dielectric materials, as dielectric beads. The plasmonic structures have to be tailored in order to generate strong field gradients necessary to trap small objects. The spatial distribution of the plasmonic particles can be adjusted using lithography methods. Their size is selected to obtain surface plasmon resonances at the wavelength of the trapping beam.

We have fabricated arrays of gold nanoparticles on top of silicon and quartz pillars, using nanosphere lithography (NSL) and etching techniques. The techniques employed permit to obtain large scale of subwavelength gold nanoparticles arranged in hexagonal and triangular arrays. The materials used have good biocompatibility and can be applied in biological applications requiring optical trapping. On the other hand, due to the optical absorption at plasmon resonances or intrinsic absorption at wavelengths below 550 nm, gold particles can serve as local heating sources.

O 63.3 Thu 11:00 H38

Nonlinear Optical Properties of Gold Thin Films by Controlled Percolation — •Stefano De Zuani, Tobias Knoblauch, Audrey Berrier, Bruno Gompf, and Martin Dressel — 1.Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

When a metal is evaporated onto an insulating substrate and the metal filling factor is gradually increased, close to the percolation the almost touching metallic particles form an almost closed film and the insulator to metal transition occurs. The optical conductivity of such ultrathin metal films is dominated by a Drude component starting at the percolation threshold in the low-frequency range and by localized surface plasmons of the isolated particles. The interplay of both components leads to a dielectric anomaly in the infrared region with a divergence of the real dielectric constant at the insulator to metal transition. We present a systematic study of the nonlinear optical properties of ultrathin gold layers around the percolation threshold in order to correlate the dielectric anomaly in the real dielectric constant to the nonlinear signal of the films. We control the approach to percolation by using metallic seeds as templates for the formation of the islands, and by pre-heating the substrates. In this way the density of the metallic clusters is kept constant. We investigate the role of the capacitive coupling of the almost touching gold clusters on the nonlinear properties of the metallic film. This work brings fundamental understanding of the nonlinear properties of ultrathin metallic films and it opens the way to an active tailoring of the nonlinear signals.

O 63.4 Thu 11:15 H38

Simulation of Plasmonic Particles with MMP — •Ueli Koch, Jens Niegemann, and Christian Hafner — Institut für Feldtheorie und Höchstfrequenztechnik (IFH), ETH Zürich, Switzerland

The Multiple Multipole Program (MMP) is a Generalized Point Matching (GPM) method using analytical multipole expansions to solve Maxwell's equations in frequency domain. MMP is a well-established and highly flexible method for the simulation of photonic nanostructures. However, for three-dimensional systems it usually requires an experienced user to position the expansions and matching points in order to model the geometry accurately. Here, we present a novel mesh-based approach, which allows simulating a large variety of geometries without user interaction. Additionally, we adapted MMP for the calculation of electron-energy loss spectra (EELS). Our implementation has been validated against analytical solutions and by comparison with results from discontinuous Galerkin time-domain (DGTD) simulations. Finally, we discuss the possibility to employ layered Green's functions, which makes MMP a powerful tool for the accurate simulation of particles on layered substrates or membranes.

O 63.5 Thu 11:30 H38

Surface Plasmons onordered and bi-continuous spongy nanoporous gold films — •Neha Sardana[1], Carsten Reinhardt[2], and Jörg Schilling[1] — [1]ZIK SiLi-nano, MLU, Halle, Germany — [2]Laser Zentrum Hannover, Hannover, Germany

In sub-wavelength optics of thin metal films (negative real dielectric constants), the dispersion relation of surface plasmons (SPs) on metal/dielectric surfaces is given as $\mathrm{k}_x{=}(\omega/c) * \sqrt[2]{[\varepsilon_m * \varepsilon_d/(\varepsilon_m + \varepsilon_d)]}$, where k_x describes the wave vector of the SP and ε_m and ε_d are the dielectric constants of the metal and dielectric resp. We investigate tuning of dispersion of SPs by keeping ε_d fixed but changing ε_m via introducing a nanoporosity into the metal. We compare a bi-continuous nanoporosity fabricated by dealloying with a uniform hexagonal porosity formed by evaporating gold Au on self-ordered nanoporous templates. The porosity leads to increase in ε_m which causes red shift of the SP frequency at constant k_x. This is observed experimentally by applying angular resolved reflection measurements. A dip in reflectivity, which shifted to shorter wavelength with increasing angle of incidence, was identified. This shift is in good agreement with effective medium theory's. Determination of SP propagating losses, was performed by leakage radiation microscopy in both direct and Fourier space. It is observed that ordered nanoporous gold film exhibits lesser scattering and overall lower attenuation than the spongy nanopores.

This metallic structure represents a bridge between designer plasmons at structured metal surfaces for microwave range and classic SP optics with plane metal layers in visible allows larger flexibility in SP devices.

O 63.6 Thu 11:45 H38

Ultrafast strong-field photoemission from plasmonic nanoparticles — •Péter Dombi[1,2], Anton Hörl[3], Péter Rácz[1], István Márton[1], Andreas Trügler[3], Joachim Krenn[3], and Ulrich Hohenester[3] — [1]Wigner Research Centre for Physics, Budapest, Hungary — [2]Max-Planck-Institut für Quantenoptik, Garching — [3]Institut für Physik, Karl-Franzens-Universität, Graz, Austria

We demonstrate strong-field electron emission from various plasmonic nanoparticles induced by ultrashort laser pulses. Significant electric field enhancement attributed to surface plasmons enable the experimental generation of up to 25-eV electrons in nano-localized fields around nanoparticles even at low exciting laser intensities. Clear correlation between the plasmonic resonance features of various nanoparticles and photoemission electron spectra are shown. The strong-field plasmonic photoemission and photoacceleration mechanisms involved are confirmed by numerical simulations.

O 63.7 Thu 12:00 H38

Tailoring the emission of electric and magnetic dipoles with plasmonic split-ring resonators — •Sven Moritz Hein and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, D-70569 Stuttgart, Germany

The radiative properties of photon emitters strongly depend on their photonic environment, i.e., on the local density of states (LDOS). Due to the high electric and magnetic fields around a resonantly excited plasmonic nanostructure, the LDOS is strongly modified. This can enhance as well as suppress both radiative and non-radiative decay rates, dependent on the location and frequency of the emitter. Using a discrete dipole approximation (DDA) algorithm, we explore the emission behavior of electric as well as magnetic dipole emitters located next to resonant split ring resonators, which are well-known for their large magnetic moment at their fundamental resonance. We also show to what extend the widely used two-dipole model of an SRR is able to explain the resulting Fano-type features in the emission spectra.

O 63.8 Thu 12:15 H38

Strong-field photoemission from nanostructures at mid-infrared frequencies — •Georg Herink, Daniel R. Solli, Sergey V. Yalunin, Lara Wimmer, Katharina Echternkamp, Max Gulde, and Claus Ropers — Materials Physics Institute and Courant Research Centre, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We investigate strong-field photoemission from plasmonic nanotips driven by ultrashort pulses at near-and mid-infrared wavelengths up to 12 μm. Kinetic energies of hundreds of electronvolts, corresponding to more than 1000 times the photon energy, are experimentally observed. The scaling of the cutoff energy with wavelength reveals electron dynamics that arise from acceleration within the enhanced optical near-field [1]. Electron dynamics and scalings exclusive to nanostructures are discussed, and their optical control is described using recent theoretical results.

[1] G. Herink, D. R. Solli, M. Gulde, C. Ropers, Nature 483,190 (2012)

O 63.9 Thu 12:30 H38

The Role of the Scattering Phase in Single Particle Spectroscopy — •Christian Dicken[1,2], Thorsten Schumacher[1,2], Daniela Ullrich[1,2], Klas Lindfors[1,2], Harald Giessen[2], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, Heisenberg Str. 1, 70560 Stuttgart, Germany — [2]4th Physics Institute, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

The continuously decreasing length scales in nanooptics and the trend towards single particle experiments requires powerful and highly sensitive measurement techniques. In many of these, such as homodyne amplification or when interferometers are used, the phase of light scattered by the nanostructure becomes important. In this talk we shed light on the properties of the scattering phase of metal nanoparticles in general and describe its strong influence on the optical response of the particle. We present an intuitive picture to understand the optical response of a metal nanoparticle as superposition of a dielectric and plasmonic contribution. Experimental data on interferometric detection of nickel nanoparticles is presented that clearly show the effects of the scattering phase and how it changes with particle size.

O 63.10 Thu 12:45 H38

Optical antennas for ultrafast spectroscopy of single CdSe nanoobjects — •Thorsten Schumacher[1,2], Daniela Ullrich[1,2], Mario Hentschel[1,2], Harald Giessen[2], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]4th Physics Institute, University of Stuttgart

Ultrafast nonlinear spectroscopy investigates the deviations from linear light-matter interaction on very short timescales. The already weak nonlinear signals are reduced further when single nanoobjects such as quantum dots, molecules, or nanoparticles are the systems of interest. We present a method to resolve ultrafast carrier dynamics of excitonic states in an individual CdSe nanowire. We observe various fast and long living effects in the transient absorption spectra that we attribute to a highly excited electron-hole plasma and excitonic state bleaching. To enhance this nonlinear response we developed a method to place gold nanoantennas in close vicinity to the nanowires. Here we present first experimental results of these hybrid systems.

O 64: Focussed Session: Solid-liquid Interfaces I

Organizers: M. Arenz (University of Copenhagen), P. Broekmann (Universität Bern), A. Flügel (BASF)

This focused session will offer an interdisciplinary discussion forum for experimental and theoretical work - including aspects in experimental and theoretical method development - in the field of electrochemical energy conversion, energy storage and nano-galvanic processes. The focus of the session is on the question what electrochemical surface science and an atomic level understanding have contributed so far and will contribute in the future to the development of new catalytic materials with advanced properties on a technological level.

Time: Thursday 10:30–13:00 Location: H31

Topical Talk O 64.1 Thu 10:30 H31

Cooperative Phenomena at the Solid/Liquid Interface — •Katharina Krischer — TU München, Germany

Complex forms of organization are often the result of nonlinear interactions between their basic building blocks. As a consequence, the system's properties cannot be explained by extrapolating knowledge about the molecular structure of the components which build up the system. Rather, in addition, information about their mutual interactions is required.

In the talk I will summarize the current state of understanding of self-organization processes occurring at the electrode|electrolyte interface with emphasis on spatial pattern formation, cooperative phenomena in ensembles of microelectrodes and non-Markovian processes at nanoelectrodes.

O 64.2 Thu 11:00 H31

Capacity of Electrochemical Interfaces — •Manuel Landstorfer and Wolfgang Dreyer — Weierstrass Institute for Applied Analysis and Stochastics (WIAS)

The differential capacity $C = dq_M/dU$, where q_M is the metal (surface) charge and U the applied potential difference between the bulk metal and the bulk electrolyte, of an electrode/electrolyte interface is unique *tool* to charactarize and investigate combinations of various electrode and electrolyte materials. Classical thermodynamic and continuum mechanical descriptions of the electrode/electrolyte interface only treat the electrolyte environment (in terms of Poisson-Boltzmann-equations and its generalizations) in the derivation of an explicit funcion $C = C(U)$ [3,4]. In contrast, we will model the interface as electrode domain Ω_M and an electrolyte domain Ω_E which share a common singular surface Σ. Based on free energy formulations for the electrolytic solution and the singular surface, as well as contact conditions for the chemical potentials, we derive explicit functions $C = C(U)$ for various types of interfaces:

- metal - dilute electrolyte - no adsorption
- metal - strong electrolyte/ionic liquid - no adsorption
- metal - electrolyte - various adsorption models

Our results are compared to experimental data which allows for a determination of model parameters in our free energy formulation.

Topical Talk O 64.3 Thu 11:15 H31

Electrochemical energy conversion - interesting challenges for Surface Scientists — •Harry E. Hoster — Technische Universität München, TUM CREATE, 10-02 CREATE Tower, Singapore 138602

I will highlight important contributions by Surface Science towards a better understanding of options and limits of improving electrodes for low-temperature fuel cells and metal-air batteries. Structure-property relationships for bimetallic electrocatalysts in fuel cells can be elegantly observed and quantified in electrochemical studies involving particularly well-defined bimetallic surfaces. Preparation and imaging methods in vacuum provide optimum control of structure and composition of such model electrodes. For typical fuel cell reactions like O_2 reduction, H_2 oxidation, or CO oxidation I will show that by this approach we can not only screen metal combinations and surface compositions for optimum performance, but also identify the roles of distinct metal surface atoms and ensembles in adsorption and reaction.

Similar to fuel cells, cathodes of metal-air batteries must be active for electrochemical oxygen reduction. The energy drawn from a metal-air cell, however, results from the formation of a solid state metal-oxide film hosted by the cathode. Using the example of a Li-O_2 model cell I will illustrate how nucleation and growth of that film can give rise to serious history dependent limitations of the available energy content.

New types of batteries also mean new challenges for Surface Scientists. We have to tackle these challenges by new efforts in developing and improving experimental and theoretical methods.

O 64.4 Thu 11:45 H31

CO Electroxidation on Pt monolayer island modified Ru(0001) electrodes — •Stephan Beckord, Albert K. Engstfeld, Sylvain Brimaud, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Bimetallic catalysts often show catalytic properties which strongly differ from those of the respective pure components. One example are PtRu catalysts, which are used, e.g., in direct methanol oxidation fuel cells (DMFC) because of their improved tolerance towards CO compared to Pt catalysts. We here report results of a study on the CO oxidation characteristics on structurally well defined PtRu bimetallic surfaces, consisting of a Ru(0001) substrate partly covered by Pt monolayer islands. To elucidate possible correlations between structure and catalytic properties, the Pt coverage was systematically varied. The surfaces were prepared by Pt evaporation under ultra high vacuum (UHV) conditions at elevated temperatures to form hexagonal islands, and characterized structurally by scanning tunneling microscopy (STM). The electrocatalytic CO oxidation was investigated in an electrochemical flow cell attached to the UHV system. In interpreting the resulting data, we take advantage of the result of earlier studies in our group on the gas phase adsorption of CO or hydrogen on similar surfaces [1], and on the electro-adsorption of hydrogen or OH on these surfaces in acid electrolyte [2]. [1] H. Hartmann et al, PCCP 14 (2012) 10919 [2] H. Hoster et al, JPC B 108 (2004) 14780

15 min. break

Topical Talk O 64.5 Thu 12:15 H31

Interaction of Pt-nanoparticles with graphitic carbon structures - a computational study — •Alexander A. Auer, Wolfgang B. Schneider, and Udo Benedikt — Max-Planck Institut für Chemische Energie Konversion

In heterogeneous electrocatalysis, often the lifetime and stability of a catalyst are the bottleneck for the performance of a catalyst. For the oxygen reduction reaction, for example, usually Pt Nanoparticles on amorphous carbon are and one degradation mechanism that is frequently observed is the detachment of nanoparticles from the support.

While the attachment of nanoparticles to carbon surfaces in electrocatalysis is interesting in itself, the question arises what the basic interaction of metallic structures and conjugated carbon structures is in general.

In this contribution we present work on the interaction of platinum nanoparticles in the size of a few atoms up to 1 nm with graphitic carbon structures, modelled by patches of graphene, using quantum chemical methods. We focus on the type and strength of interaction as well as the possibility to increase adhesive forces. Fruthermore, some insights will be discussed on how electrochemical reactions can be modelled using quantum chemical methods including the electrochemical potential and explicit or implicit representations of the solvent.

O 64.6 Thu 12:45 H31

Interfacial water properties at room temperature: a comparison between PBE and RPBE-D3 — •Tanglaw Roman and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

In studying the properties of solid-liquid interfaces at ambient temperature, using ab initio molecular dynamics (AIMD) is advantageous because of its reliable description of metal-water interaction. In this talk we will be discussing results of investigations motivated by the suggestion that the dispersion-corrected RPBE functional (RPBE-D3) gives a more reasonable description of both the intermolecular water-water and water-metal interaction, compared with the more popular PBE functional [1]. More specifically, we point out differences between PBE and RPBE-D3 results for room-temperature interfacial water structure on three surfaces: (1) ideal Pt(111), (2) pseudomorphic Ru monolayer on Pt, on which water more strongly adsorbs, and (3) hydrogen-covered Pt, on which water more weakly adsorbs [2]. Three trajectories are used for each case, made distinct by how the interfacial bilayer is initially configured: H-up, H-down, and completely random in terms of both water molecule positions on the Pt surface and molecular orientation.

[1] K. Tonigold, A. Groß, J. Computational Chem. 33 (2012) 695.

[2] T. Roman, A. Groß, Catalysis Today, in press.

O 65: Surface and Interface Magnetism II (jointly with MA)

Time: Thursday 10:30–13:00 Location: H33

O 65.1 Thu 10:30 H33

Deviation from Coulombic behavior in short-range interactions of atoms on the GaAs(110) surface — •David Gohlke[1,2] and Jay Gupta[1] — [1]Ohio State University, Columbus, OH USA — [2]Universität Regensburg, Regensburg, Germany

Mn-doped GaAs is a prototypical dilute magnetic semiconductor where substitutional Mn act as electron acceptors while their magnetic moment allows for long-range magnetic interactions. By using low-temperature (5K) scanning tunneling microscopy (STM), we examine the electronic properties of individual Mn dopants in GaAs. We have previously shown that the binding energy of the Mn electron acceptor state can be tuned by controlled atomic-scale placement of a nearby charged defect, and that the shift of the binding energy due to repulsion between the bound hole and these charged defects follows a 1/r Coulombic behavior [Lee and Gupta, Science (2010), Gohlke et al., submitted]. Here we will discuss our observations of deviations from the 1/r behavior. First, our data show that the anisotropy of the GaAs(110) surface affects the interaction between Mn acceptors and charged adatoms. Second, for charged defects brought within 2nm of the acceptor, we observe defect-induced band bending that changes the occupancy of a hybridized Mn state located in the valence band, resulting in a turnaround behavior of the measured resonance energy.

This research has implications in studying the interactions between atoms in Mn-doped GaAs, a material for which the mechanisms for magnetism are still debated.

O 65.2 Thu 10:45 H33

Mapping of the spin-resolved band structure of fct cobalt films on Cu(100) — •Christian Tusche[1], Martin Ellguth[1], Alexander Krasyuk[1], Carsten Wiemann[2], Vitaliy Feyer[2], Marten Patt[2], Claus M. Schneider[2], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany — [2]Forschungszentrum Jülich, 52428 Jülich, Germany

We report on the spin resolved band structure of ultra thin fct cobalt films grown on Cu(100), measured over large volumes in momentum space. Experiments were carried out at the NanoESCA beamline [1] of the Elettra synchrotron. The instrument, consisting of a photoelectron microscope and an imaging energy analyzer, directly maps the parallel momentum component of photoelectrons at a fixed energy. An imaging spin filter, based on the reflection of low energy electrons at a W(100) crystal, was installed temporarily at the exit of the energy filter [2]. This allowed to record the spin polarization at $4 \cdot 10^3$ discrete reciprocal space points, in each momentum image. This efficient approach gives direct access to majority and minority spin bands in the Fermi surface and their dispersion towards larger binding energies. Using 40 eV to 200 eV photons, several constant energy cuts in the 3D Brillouin zone are selected. The comprehensive data sets are expected to serve as valuable input for advanced concepts in theory for the refined treatment of spin-dependent electron correlation. — [1] Wiemann, Patt, Krug, Weber, Escher, Merkel, Schneider, e-J. Surf. Sci. Nanotech. **9**, 395 (2011) — [2] Tusche, Ellguth, Ünal, Chiang, Winkelmann, Krasyuk, Hahn, Schönhense, Kirschner, Appl. Phys. Lett. **99**, 032505 (2011)

O 65.3 Thu 11:00 H33

Investigation of the Si/Fe interface with standing-wave excited HAXPES — •Sven Döring[1], Michael Voigt[2], Martina Müller[2], Mihaela Gorgoi[3], Daniel E. Bürgler[2], and Claus M. Schneider[1,2] — [1]Experimentalphysik, Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [2]PGI-6, Forschungszentrum Jülich, 52425 Jülich — [3]Helmholtz Zentrum Berlin für Materialien und Energie, Albert Einstein Str. 15, 12489 Berlin

The interface between the ferromagnet Fe and the semiconductor Si is supposed to be a crucial part of future spintronic devices. The possible formation of silicides and the degree of an intermixing between the layers at the interface has a large influence on the conductance and efficiency of spin-injecting currents from the metal layer into the semiconductor. Therefore, we studied the interface between thin MBE-grown layers of Si on Fe with standing-wave excited hard x-ray photoemission spectroscopy. This method gives us a chemically sensitive depth-profile of the sample with a depth-resolution of a few Å and we are able to compare the interface structure of samples that were grown under different conditions.

The Si/Fe sample systems were grown on top of multilayer mirrors that give rise to a high reflectivity and thus to strong modulations of the HAXPES signals. The Fe layer was grown as a wedge which enables us to perform rocking-curve experiments as well as so-called Swedge scans.

O 65.4 Thu 11:15 H33

Inverse proximity effects in superconductor/ferromagnet bilayer explored by polarized neutron reflectometry — •Yury Khaydukov[1], Bela Nagy[2], Jung-Hwa Kim[1], Thomas Keller[1], Laszlo Bottyan[2], and Bernhard Keimer[1] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]Wigner Research Centre for Physics, Budapest, Hungary

The inverse proximity effect, i.e. the appearance of magnetic correlations in the superconductor (S) close to the interface with a ferromagnet (F) was first considered theoretically in early 2000s. The origin of this effect is the exchange coupling of free (itinerant) electrons near the S/F interface. The spin up electron of a Cooper pair would prefer to be located in ferromagnetic region while spin down electrons would remain in the superconducting region This leads to the development of a magnetic sublayer within the S layer close to the interface with its magnetization antiparallel to the magnetization of free electrons of F layer Me. Thickness of the sublayer is comparable with the superconducting coherence length, ξ. We studied the effect using different methods including transport measurements, SQUID magnetometry etc. However, the main method which allowed us to get the information about the thickness of proximity induced magnetic sublayer was Polarized Neutron Reflectometry . Dependence of this effect (sign and size) on the temperature, coherence length of the S layer ξ, exchange coupling strength of the F layer will be discussed in details.

O 65.5 Thu 11:30 H33

Spin-density wafe node on antiferromagnetic Cr(110) islands — •Tobias Mauerer[1], Pin-Jui Hsu[1], Weida Wu[2], and Matthias Bode[1] — [1]Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg — [2]Department of Physics and Astronomy and Rutgers Center for Emergent Materials, Rutgers University, Piscataway, New Jersy 08854, USA

We have performed a detailed analysis of the evolution of the charge-density wave (CDW) on the surface of nanoscale Cr islands grown on W(110). By combining conventional spin-averaged and spin-polarized scanning tunneling microscopy (SP-STM) we show that the CDW wavelength exhibits a striking thickness dependence. In particular, the CDW wavelength along the surface $[1\bar{1}0]$ direction increases by about 30% as the island thickness is decreased from about 50 nm to 5.2 nm. A gap with no CDW visible at the island surface appears for films within the thickness range of $3.7 \leq \Theta \leq 5.2$ nm. At even lower film thickness the CDW reappears until it vanishes at $\Theta \leq 2.5$ nm By applying SP-STM we show that the Cr surface is non-magnetic within the CDW gap. The CDW gap and the thickness dependence is explained in terms of a reorientation of the SDW vector $\mathbf{Q}$, which rotates from bulk-like $\langle 001 \rangle$ directions into the [110] surface normal. We propose that the SDW pins with a node at the island surface, resulting in a vanishing surface magnetic moment.

O 65.6 Thu 11:45 H33

Scanning tunneling microscopy and spectroscopy of MnPc on noble metal (111) surfaces — •Jens Kügel, Jeannette Kemmer, Pin-Jui Hsu, and Matthias Bode — Institute of Experimental Physics II, University Würzburg, Germany

The growth, electronic structure, and magnetic excitations of transition metal phthalocyanine (TM-Pc) molecules adsorbed on noble metal fcc(111) substrates have recently attracted considerable interest. While phthalocyanines with a central ion consisting of Fe, Co, Ni, and Cu have already been studied extensively, only few studies deal with MnPc, even though this molecule carries the highest net magnetic moment in the gas phase ($S = 3/2$) [1]. This property makes it a promising candidate for the observation of collective interaction phenomena with the substrate, such as the Kondo effect. In this contribution we present low-temperature ($T = 5$ K) scanning tunneling microscopy and spectroscopy data of Mn-Pc adsorbed on Au(111) and Cu(111). The tunneling spectra of Mn-Pc show a distinctly asymmetric conductance around the Fermi level. Our results indicate that this feature critically depends on the chemical state of the tip. By systematically modifying the coupling strength between the molecule and the substrate we will discuss under which conditions the Kondo effect can be observed.

[1] A. Stróżecka *et al.*, Phys. Rev. Lett. **109**, 147202 (2012)

O 65.7 Thu 12:00 H33

Spin-resolved measurements of single molecular magnets on graphene — •Jens Brede, Maciej Bazarnik, Régis Decker, Jörg Schwöbel, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, 20355 Hamburg, Germany

The use of magnetic molecules opens a gateway to a flexible design of novel spintronic devices to store, manipulate, and read spin information at the nanoscale. Crucial is the precise knowledge of molecular properties at the interface towards an electrode. Progress in this field relies on resolving and understanding the physics at the relevant interfaces. In particular the role of individual molecular constituents and the impact of the atomic environment on molecular properties, determine device relevant parameters, such as conductance and spin polarization. Recently, the incorporation of a graphene sheet to electronically decouple molecules from a ferromagnetic surface was addressed by surface averaging techniques.

Here, we applied spin-polarized scanning tunneling microscopy to resolve the physics of the molecule-graphene-ferromagnet interface. The analysis focuses on different phthalocyanine molecules adsorbed on cobalt intercalated graphene on Ir(111). The phthalocyanine constitutes of an organic macrocyclic ligand and can be functionalized with various metal ions in order to modify, e.g. the molecular spin state. We will discuss the spin-dependent transport from magnetic surfaces through such molecules. In particular, the spin polarizations of molecular frontier orbitals are resolved with sub-molecular spatial resolution and the variations in the lifetimes of different states are discussed.

O 65.8 Thu 12:15 H33

Chemically programmable 2D electron spin arrays — Christian Wäckerlin[1], •Jan Nowakowski[1], Shi-Xia Liu[2], Michael Jaggi[2], Jan Girovsky[1], Dorota Siewert[1], Aneliia Shchyrba[3], Tatjana Hählen[1], Armin Kleibert[1], Peter M. Oppeneer[4], Frithjof Nolting[1], Silvio Decurtins[2], Thomas A. Jung[1], and Nirmalya Ballav[5] — [1]Paul Scherrer Institute, Switzerland — [2]University of Bern, Switzerland — [3]University of Basel, Switzerland — [4]Uppsala University, Sweden — [5]Institute of Science Education and Research, Pune, India

Spin-bearing metal-organic complexes on ferromagnetic substrates are interesting model-systems which allow studying the magnetism of individual magnetic ions in the proximity of a ferromagnetic metal. In our most recent work we have employed synthetically directed self-assembly to fabricate a highly ordered, two-dimensional chessboard-like supramolecular structure of Fe and Mn building-blocks which is exchange-coupled to a suitable ferromagnetic substrate. On-surface coordination-chemistry is then used to selectively control the spin-states in the resultant Fe-Mn-Fe spin-array. We have combined Scanning Tunneling Microscopy (STM) and X-ray Magnetic Circular Dichroism (XMCD) experiments which provide local/spatially averaged and element-specific information, respectively. High resolution STM also yields direct visualization of the axial ligands at the phthalocyanine cores.

O 65.9 Thu 12:30 H33

Modifying the magnetic properties of adsorbed spin bearing porphyrins by chemical stimuli — •Jan Girovsky[1], Christian Wäckerlin[1], Kartick Tarafder[2], Jan Nowakowski[1], Dorota Siewert[1], Tatjana Hählen[1], Aneliia Shchyrba[3], Armin Kleibert[1], Frithjof Nolting[1], Thomas A. Jung[1], Peter M. Oppeneer[2], and Nirmalya Ballav[4] — [1]Paul Scherrer Institut, Switzerland — [2]Uppsala University, Sweden — [3]Universtity of Basel, Switzerland — [4]Indian Institute of Science Education and Research (IISER-Pune), India

Metalloporphyrins adsorbed on and exchange coupled to ferromagnetic substrates [1], have been stimulated by different axial ligands like NO and NH3. Beyond the modification of the electronic states in the ad-molecule by the chemical ligation [2], we now focus on the sign and strength of the exchange interaction with the substrate [3,4]. In our experimental (XMCD, STM, XPS) and theoretical (DFT+U) work we provide evidence for cooperativity between the axial ligand on top and the surface ligand below the porphyrin (”surface spin trans effect”). We present four magneto-chemical effects: reduction (HS → IS), quenching ($S \neq 0 \rightarrow S{=}0$), flipping (”$S > 0$” → ”$S < 0$”) and induction ($S = 0 \rightarrow S \neq 0$) of magnetic moments in specific ad-porphyrins upon coordination with different chemical ligands.

[1] A. Scheybal et al, Chem Phys Lett 411, 214 (2005).
[2] W. Hieringer et al, J Am Chem Soc 133, 6206 (2011).
[3] C. Wäckerlin et al, Nat Comms 1, 61 (2010).
[4] C. Wäckerlin et al, Chem. Science 3, 3154 (2012).

O 65.10 Thu 12:45 H33

Structural and magnetic properties of pyridyl and benzonitrile based metal-organic networks — •Tobias R. Umbach[1], Matthias Bernien[1], Claudia Hartmann[1], Alexander Krüger[1], Janina N. Ladenthin[1], Constantin Czekelius[2], Jose I. Pascual[1,3], Katharina J. Franke[1], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Chemie und Biochemie - Organische Chemie, Freie Universität Berlin Takustr. 3, 14195, Berlin, Germany — [3]CIC nanoGUNE Consolider, Tolosa Hiribidea, 76, E-20018 Donostia , San Sebastian, Spain

Metal-organic networks offer the possibility to tune the electronic and magnetic functionality of surfaces on a nanometer scale. Here we use LT-STM to characterize the structure of metal-organic networks of transition metal atoms (Co, Fe) and triangular organic linkers, which exhibit either three pyridyl or three benzonitrile endgroups on Au(111). In the case of benzonitrile endgroups, the mixture with transition metal atoms leads to the formation of self-assembled ordered networks with a honeycomb structure. Every transition metal atom is surrounded by three benzonitrile groups forming three-fold coordination nodes. By changing the endgroups to pyridyl, the coordination motif changes significantly. The transition metal atoms exhibit the same in-plane coordination scheme with an additional molecule centered on top. The magnetic properties of the networks are investigated by XMCD measurements, which reveal that, despite their different structures, they all exhibit sizable magnetic moments and magnetic anisotropy.

O 66: Oxide Surfaces II

Time: Thursday 10:30–13:15 Location: H42

O 66.1 Thu 10:30 H42

Atomic-scale insights into geometrical and electronic properties of the N3 dye on TiO2 anatase (101) — •C. S. Kley[1], C. Dette[1], S. J. Jung[1], G. Rinke[1], J. Cechal[1], S. Rauschenbach[1], C. Patrick[2], F. Giustino[2], S. Stepanow[1], and K. Kern[1,3] — [1]MPI for Solid State Research, Stuttgart, DE — [2]University of Oxford, Department of Materials, Oxford, UK — [3]EPFL, Institut de Physique de la Matiere Condensee, Lausanne, CH

Dye-sensitized solar cells (DSSCs) constitute a promising approach to sustainable and low-cost energy production with considerable light conversion efficiencies. Among many efforts, the understanding of the dye adsorption geometry, its electronic alignment and mutual lateral interaction is of paramount importance to optimize the photovoltaic performance of DSSCs. Here, we study the geometric and electronic properties of N3 dye molecules on the TiO2 anatase (101) surface by means of scanning tunneling microscopy and spectroscopy methods in UHV. Electrospray ion beam deposition is employed to deposit the thermally fragile photosensitizer onto the substrate. In contrast to theoretical predictions suggesting a specific thermodynamically most stable N3 adsorption configuration, our studies reveal variable N3 adsorption geometries on the TiO2 anatase (101) surface. The role of kinetics, photosensitizer ionization and substrate defects will be discussed and additional studies of the N3 anchor ligand BINA will be correlated to our findings. Further, the electronic configuration of the adsorbed N3 molecules will be presented. Our experimental results are supported by first-principle DFT based calculations.

O 66.2 Thu 10:45 H42

Carboxylic acid on all stable TiO_2 rutile surfaces: Comparison of DFT and DFTB potentials — •Wolfgang Heckel, Beatrix Elsner, and Stefan Müller — Hamburg University of Technology, Institute of Advanced Ceramics, Denickestr. 15, D-21073 Hamburg

In order to control the mechanical properties of hybrid materials, the detailed knowledge of the interfaces, the atomic structure and stability is crucial. Both methods, density functional theory (DFT) and density functional based tight binding (DFTB) allow for the investigation of the local electronic structure and the determination of desired observables like binding energy, while growing further towards about 5-10 times larger model systems with the latter.

As a prototype adsorbate we tested acetic acid on TiO_2 (110), (011) and (100) surfaces for two DFT exchange-correlation functionals (PBE and PBEsol) and for DFTB being able to estimate the accuracy of results for arbitrary adsorbates in the future.

We put the focus on the ability of the methods to describe correctly the role of the carboxylic hydrogen ion, which dissociates during adsorption and forms an OH species stabilizing the adsorption, as shown in experiments (e. g. [1]). All methods applied prefer the dissociated adsorption mode to the molecular mode, however the results differ about prefering acetic acid or acetate.

Supported by DFG, SFB 986, project A4.

[1] Sayago et al., J. Phys. Chem. B **108**, 14316 (2004)

O 66.3 Thu 11:00 H42

Photodesorption in the CO/TiO_2-system — •Hendrik Spieker and Thorsten Klüner — Theoretical Chemistry, Carl von Ossietzky Universität, PO Box 2503, 26111 Oldenburg

Due to its high photocatalytic activity, titanium dioxide is of application-oriented interest. Unfortunately, the fundamental mechanisms of surface chemistry are completely unknown. The adsorbate-substrate-system CO/TiO$_2$(110) has recently been studied as a model system concerning a fundamental understanding of adsorption and desorption phenomena. [1]

Making use of an embedded cluster approach, two- and three-dimensional potential energy surfaces (PES) for the ground state and relevant excited states of the CO molecule are calculated on a post Hartree-Fock level of theory. These PES serve as potentials for quantum dynamical stochastic wave packet studies, yielding quantum state resolved final state product distributions. Furthermore, the desorption mechanism for the CO molecule interacting with a TiO$_2$(110)-surface in consequence of a vertical excitation will be elucidated in detail. Concerning these results, the correction of the basis set superposition error within the quantum chemical calculations is found to be essential.

[1] M. Mehring, T. Klüner, *Chem. Phys. Lett.* **513**, 212-217 (2011).

O 66.4 Thu 11:15 H42

Ab initio calculations on the adsorption energy of NO on TiO$_2$(110) — •Marie Arndt and Thorsten Klüner — Theoretische Chemie, Carl von Ossietzky Universität Oldenburg, Germany

Photocatalytic reactions on metaloxide surfaces are an important section in technical industries. An outstanding photocatalyst is the semiconductor titaniumdioxide. In this context, the adsorption and desorption processes of small molecules on the substrate surfaces play an important role in theoretical and experimental analysis. This study focuses on the characterization of the adsorption of NO on a rutile(110) surface. We investigated the adsorption by using ab initio calculations, such as restricted open shell Hartree-Fock and restricted open shell Møller-Plesset second order perturbation theory. To describe the electronic ground state of this open shell system, an embedded cluster model of the type $\mathrm{Ti_9O_{18}Mg_7^{14+}}$ was used. Using the *Molcas*[1] quantum chemistry package, the goal is to find the global minimum of the adsorption energy. Within our model, six degrees of freedom of our diatomic NO molecule on a rigid TiO$_2$ surface are defined. In this study, we varied the desorption coordinate z and the polar angle θ, by keeping the lateral coordinates x and y, the azimuthal angle φ and the NO bond length r fixed. The preferred orientation of NO on the rutile(110) surface has been found by modeling a 2D potential energy surface and is discussed in terms of a molecular orbital picture. The results revealed a tilted orientation of the NO at a distance of 3.0 Å to the surface. [1] Division of Theoretical Chemistry, Molcas 7.6, Lund University, 2011.

O 66.5 Thu 11:30 H42

Co-Salen on NaCl(001) and NiO(001): Substrate influence on adsorption geometry and growth — •Josef Grenz[1], Alexander Schwarz[1], David Gao[2], Matthew Watkins[2], Alexander Shluger[2], and Roland Wiesendanger[1] — [1]Inst. of Ap. Phy., University of Hamburg, Germany — [2]University College London, UK

By depositing the same molecule, i.e., Co-Salen, on two chemically different substrates, i.e., NaCl(001) and NiO(001), with the same surface structure disparities as well as equalities regarding adsorption geometry and growth were investigated.

Since these materials are bulk insulaters, atomic force microscopy in the non-contact mode operated was applied to simulataneously resolve the atomic structure of the surface and to image individual molecules. On both ionic substrates the molecule adsorbs on top of the anions, i.e., chlorine and oxygen. However, on NaCl(001) 16 stable orienations are observed [1], while only 8 are present on NiO(001). Moreover, tip-induced translational motion of individual Co-Salen molecules occur along preferred crystallographic directions and coincide with stable orientations of the molecule on the respective substrate. Tip-induced motions are more frequent on NaCl(001) than on NiO(001), indicating a larger binding energy on the latter. This presumption is supported by the initial layer-by-layer growth observed on NiO(001), while island growth is observed on NaCl(001) [2]. All these experimental findings are in agreement with density functional theory (DFT) calculations.

[1] K. Lämmle, *et al.*, Nano Lett. **10**, 2965-2971 (2010).

[2] S. Fremy, *et al.*, Nanotechnology **20**, 405608 (2009).

O 66.6 Thu 11:45 H42

Boron nitride as a template for molecular adsorption, self-assembly and electronic decoupling of the prototype macrocycle porphine. — •Felix Bischoff, Sushobhan Joshi, Knud Seufert, David Ecija, Saranyan Vijayaraghavan, Willi Auwärter, and Johannes Barth — Physik Department E20, TUM, James Franck Str. 1, 85748 Garching, Germany

Motivated by its bulk and thin film properties and successful incorporation into graphene nanodevices, boron nitride (BN) has gained great attention. Recently, a vapor-deposited BN monolayer on a Cu support was comprehensively characterized [1]. It is topographically smooth, yet electronically patterned and therefore provides a versatile template for molecular adsorption, self-assembly and electronic decoupling of molecular nanosystems. In this work, these properties are exemplified by systematic STM and STS experiments. The macrocyclic model compound porphine (2H-P) does not spontaneously form ordered structures on bare Cu at room temperature due to strong substrate-adsorbate interactions. However, a BN spacer layer electronically decouples these molecules and enables 2-D self-assembly. It also serves as an electronic template due to variations in its potential landscape and traps 2H-P at specific sites. At low- and intermediate coverages, arrays of well-separated, but highly-ordered porphine islands are observed, following the BN moiré structure. The inhomogenous BN template also dictates the electronic level alignment, as evidenced by a spatial modulation of the energy of porphine frontier orbitals.

[1] Joshi et al., Nano Lett., 2012, 12 (11), pp 5821-5828

O 66.7 Thu 12:00 H42

Single molecules in a petri dish: Iodine dissociation of CHP on a hexagonal boron nitride monolayer — •Thomas Dienel[1], Roland Widmer[1], Ari P. Seitsonen[2], Jürg Hutter[2], and Oliver Gröning[1] — [1]nanotech@surfaces Lab, Empa, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland — [2]Physical Chemistry Institute, University of Zurich, CH-8057 Zurich, Switzerland

Well-defined monolayers of hexagonal boron nitride (h-BN) can be produced by thermal decomposition of borazine (HBNH)$_3$ on transition metal surfaces. On Rh(111) a strongly corrugated superstructure of depressions with a periodicity of 3.22nm is formed. There weakly bonded h-BN regions called "wires" separate strongly bonded "pores" with a diameter of 1.5nm, where organic molecules can be efficiently trapped[1]. We report on the adsorption behavior and properties of hexaiodo-substituted macrocycle cyclohexa-m-phenylene (CHP) on corrugated h-BN. The CHP molecules adsorb within the pores and are aligned in [12] direction of the superstructure reflecting the inner structure of the h-BN monolayer. The terminal iodine atoms of the CHP can be dissociated by thermal annealing [2, 3]. Contrary to the case on metals, the h-BN substrate imposes a distinct abstraction sequence, which we follow in situ by scanning tunneling microscopy and DFT calculations. With these insights to the catalytic properties of h-BN we pave the road to bottom-up fabrication of graphene by aryl-aryl coupling on h-BN. [1] S. Berner et al., Angew. Chem. Int. Ed. 46 (2007) 5115. [2] M. Bieri et al., Chem. Commun., 45 (2009) 6919. [3] M. Bieri et al., JACS , 132 (2010) 16669.

O 66.8 Thu 12:15 H42

Stability of self-assembled organic monolayers on ZnO — •Philipp Herrmann and Georg Heimel — Institut für Physik, Humboldt Universität zu Berlin, Germany

Its wide bandgap and natural abundance make ZnO a promising material for optoelectronic devices. Particulary tempting is the use of ZnO in conjunction with organic semiconductors, but this requires detailed information on the interfaces in such hybrid systems. Given the complex phase diagram of ZnO surfaces, reliable means to control the interfacial properties are needed for real applications.

We therefore explore the functionalization of ZnO surfaces with self-assembled monolayers (SAMs) of covalently attached organic molecules. The stability of these SAMs against water and oxygen is investigated by first-principles thermodynamics based on periodic density functional theory calculations.

Once an effective docking chemistry is found, these SAM molecules can be chemically modified with dipolar docking groups to control the alignment between the electronic levels of ZnO and a subsequently deposited organic semiconductor.

O 66.9 Thu 12:30 H42

Diffusion and Reaction on ZnO surfaces — •Navid Abedi and Georg Heimel — Institut für Physik, Humboldt-Universität zu Berlin, Brook-Taylor Straße 6, 12489 Berlin, Germany

In an attempt to develop a systematic strategy for the concomitant stabilization and functionalization of ZnO surfaces, we computationally explore the formation of self-assembled monolayers (SAMs) of covalently attached organic molecules. To this end, we perform density functional theory (DFT) based periodic band-structure calculation and use the nudged elastic band (NEB) method to study reaction barriers and -paths as well as transition states on ZnO surfaces. Particular emphasis has been put on hydrogen, oxygen, and hydroxide diffusion, as well as water and methanol dissociation. From these results we derive guidelines for the design of kinetically stabilized SAMs which can subsequently be modified to tune surface properties.

O 66.10 Thu 12:45 H42

Density Functional Theory study of adatom adsorption on metal supported thin Zirconia films — •Wernfried Mayr-Schmölzer, Florian Mittendorfer, and Josef Redinger — Center of Computational Materials Science, Technical University of Vienna, Austria

Zirconium dioxide is a material with many interesting properties, which make it useful for various technological applications, for example as a solid electrolyte in solid-oxide fuel-cells or as an oxygen gas sensor.

We present the results of DFT calculations of the interface between thin zirconium oxide films and supporting metals like Pt_3Zr and Pd_3Zr. Both substrates are very stable and can be used to experimentally grow thin ZrO_2 films by oxidation. Using the Vienna Ab-initio Simulation Package (VASP) employing both standard PBE and van-der-Waals density functionals a thorough investigation of the structural and electronic properties was done of both small model cells and the experimentally found large super cells. Furthermore the changes induced by oxygen vacancies were studied. The ground state structure was confirmed by simulation of the resulting core level spectra.

Additionally we investigated the adsorption of late transition metals such as Gold or Nickel on the supported zirconium oxide film. Furthermore the behavior of water molecules on the surface generated by the thin Zirconia film was investigated.

This work has been supported by the Austrian Science Fund under the project number F4511-N16.

O 66.11 Thu 13:00 H42

Ab Intio Study of Amino Acid Adsorption on ZnO (10-10) — •Svea grosse Holthaus, Susan Köppen, Thomas Frauenheim, and Lucio Colombi Ciacchi — University of Bremen, Bremen Center for Computational Material Science

In a recent study the toxicity of ZnO nanoparticles towards mammalian cells was found to be directly related to particle dissolution causing an uptake of particle remnants and toxic Zn{2+} ions into the cell. In this context the release of Zn{2+} ions was found to be different in cell culture media containing various amino acids [1]. The adsorption of different amino acids on ZnO constitutes a first step in describing the overall solid liquid interface of a nanoparticle in a biological environment.

In our study the adsorption of two charged (Argenine, Glutamic Acid) and three polar (Serin, Cystein, Glutamine) amino acids on ZnO(10-10) embedded in water are investigated using ab initio molecular dynamics simulations. An analysis of the obtained dynamics implies that the ampholytic backbone forms bond to the first water layer. Furthermore the presence of the amino acid is seen to influence the hydroxylation of the first water layer compared to pure surface water systems. Depending on the local water structure surrounding the back bone amino group, a hydrogen transfer to the first water layer is observed.

[1] Xia,T.;Kovochich,M.;Liong,M.;Mädler,L.;Gilbert,B.;Shi, H.; Yeh, J. I.; Zink, J. I.; Nel, A. E. ACS Nano 2008, 2, 2121-2134.

O 67: Competition for the Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00 Location: H45

O 67.1 Thu 10:30 H45

Magnon Rashba effect at ferromagnetic surfaces — •Khalil Zakeri Lori — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Rashba effect refers to as a spin–splitting phenomenon of the electronic band structure in the absence of any external magnetic field. It originates from a fundamental effect known as spin–orbit coupling. Basically, the relativistic motion of electrons produces a magnetic field, which couples to their spins and causes a splitting in the energy levels of electrons with different spins. It offers a way to control and manipulate the electrons spin and thus lies in the central idea of spintronics. We report a similar effect on the spin integer quasi-particles i.e. magnons at a ferromagnetic surface. We provide the first direct experimental evidence, which demonstrates that the dispersion relation of surface magnons in the presence of spin–orbit coupling and in the absence of time-reversal symmetry shows a splitting for different magnetization directions, similar to the electron dispersion relation at metal surfaces [1]. Moreover, we will show that the lifetime, amplitude, group and phase velocity of surface magnons propagating along two opposite (but equivalent) directions perpendicular to the magnetization are different [2]. Our findings can inspire ideas for designing new spintronic devices based on this new effect. [1] Zakeri *et al.*, Phys. Rev. Lett. **104**, 137203 (2010). [2] Zakeri *et al.*, Phys. Rev. Lett. **108**, 197205 (2012).

O 67.2 Thu 11:00 H45

Emergent quantum size effects at surfaces of correlated and topological solids — •Phil King — Kavli Institute for Nanoscale Science, Cornell University, USA

We use angle-resolved photoemission (ARPES) to probe quantum-confined electron systems created, at the surfaces of correlated oxides and topological insulators, by control of surface charge. In transition-metal oxides, we write this directly by forming surface oxygen vacancies through UV light irradiation. We use ARPES to image the *d*-electron subband ladder of the resulting oxide two-dimensional electron liquids, revealing a delicate interplay between quantum-confinement, orbital ordering, spin-orbit interactions and electronic correlations.[1,2] In topological insulators, we show that creation of similar surface quantum wells leads to a hierarchy of electronic states with simultaneous confinement of electron- and hole-like subbands,[3−5] the former showing giant tuneable Rashba spin splittings.[4,5] We uncover a complex band and binding energy dependence of the coupled spin-orbital texture of this surface electronic system through circular dichroism in ARPES. We show how this results from a novel connectivity between quantum well and topological surface states, enforced by the topologically non-trivial nature of the host system.[5] Together, these studies reveal the drastic reconstruction of electronic structure that occurs from electric field-induced confinement across a variety of emerging quantum materials. [1] Nature Mat. 10 (2011) 114; [2] Phys. Rev. Lett. 108 (2012) 117602; [3] Nature Commun. 1 (2010) 128; [4] Phys. Rev. Lett. 107 (2011) 096802; [5] Nature Commun. 3 (2012) 1159.

O 67.3 Thu 11:30 H45

Comparative Density Functional Theory Study of Acetaldehyde Hydrodeoxygenation Mechanisms on Ru and RuO_2 Catalysts — •Lars Grabow — Chemical and Biomolecular Engineering, University of Houston, 4800 Calhoun Rd., S222, Houston, TX 77204-4004

The hydrodeoxygenation (HDO) mechanism of acetaldehyde, a surrogate molecule for the over 400 different oxygenated species in biomass-derived pyrolysis oil, is presented for the Ru(0001) and RuO_2(110) surfaces based on Density Functional Theory results. Under typical HDO reaction conditions, the thermodynamic phase diagram indicates that the RuO_2(110) surface is partially reduced and terminated by OH-groups on the bridging O-sites. Further reduction and creation of a surface O-vacancy site are necessary to create an active site for acetaldehyde adsorption through its terminal O-atom and selective conversion to ethylene. In contrast, acetaldehyde is more easily activated on Ru(0001), but metallic Ru favors C-C bond over C-O bond scission which leads to the unwanted formation of CO and CH_4. Given the higher C-O bond scission selectivity on the metal-oxide, a rapid prediction method for surface phase diagrams and equilibrium O-vacancy concentrations of other rutile(110) surfaces is developed. In combination with a more detailed understanding of the HDO mechanism on metal and metal-oxide catalysts this model can be used for the development of new and efficient catalysts that can lead to an increased utilization of biofuels.

O 67.4 Thu 12:00 H45

Controlling the Conformation of Peptides and Proteins on Solid Surfaces in Ultrahigh Vacuum — •Stephan Rauschenbach — Max-Planck-Institute for Solid State Reseach, Stuttgart

The hierarchical self-assembly of functional proteins through folding is a versatile and robust approach to generate functional nanoscale structures. It can, however, not be mimicked outside of biological systems.

We developed an electrospray ion beam deposition (ES-IBD) system capable of depositing nonvolatile molecules including proteins and polypeptides on surfaces in ultrahigh vacuum (UHV). In this environment we study their structure and electronic properties with resolution at the atomic level using scanning tunneling microscopy (STM).

We show that the structure of polypeptides adsorbed on a surface can be controlled on several length scales, using features unique to ES-IBD. Bradykinin, a short peptide of 9 amino acids (AA) folds into an equilibrium structure, influenced by the molecule-substrate interaction. Long polypeptide chains (unfolded cytochrome-c, 104 AA) do not reach an thermal equilibrium, but instated fold randomly, perfectly following polymer statistics in two dimensions (2d). In this case, ES-IBD allows us to select the mechanical properties of the gas phase ion before deposition and steer the structure on the surface between extended chains for high charge states and refolded 2d-random coils for low charge states.

This result shows that ES-IBD combined with high resolution UHV STM, opens the door to conformational control of 2d polypeptides and its application to rationally fold functional nanostructures at surfaces.

O 67.5 Thu 12:30 H45

Surface-aligned femtochemistry: Uni- and bimolecular reaction dynamics on oxide surfaces — •Mihai E. Vaida[1], Thorsten M. Bernhardt[2], and Stephen R. Leone[1] — [1]Departments of Chemistry and Physics, University of California and Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States — [2]Institute of Surface Chemistry and Catalysis, University of Ulm, 89069 Ulm, Germany

The breaking and making of chemical bonds in molecules attached to a substrate constitute the elementary steps of surface chemical reactions and occur on the ultrafast time scale of nuclear motion. Their understanding is fundamental to the molecular level conception of chemical reaction mechanisms on surfaces, especially, for example, in catalytic materials. In this contribution a combination of an optical pump-probe configuration with time-of-flight mass spectrometry is employed to monitor in real time the mass and the relative velocity of intermediates and products of photoinduced surface reactions. Results are presented for the application of this technique to the photodissociation dynamics of methyl iodide and methyl bromide as well as to the formation dynamics of iodine, bromine and iodine monobromide molecules on magnesia ultrathin films on a Mo(100) single crystal surface. A new perspective and a further improvement of the experimental procedure will also be presented regarding the study of surface chemical reactions with femtosecond high order harmonic vacuum ultraviolet and extreme ultraviolet laser pulses by core level photoemission spectroscopy and mass spectrometry.

O 68: Graphene: Preparation and Characterization I (jointly with HL, MA and TT)

Time: Thursday 10:30–13:15 Location: H17

O 68.1 Thu 10:30 H17

Synthesis of graphene on $(6\sqrt{3} \times 6\sqrt{3})$R30° reconstructed SiC surfaces by molecular beam epitaxy — •Timo Schumann[1], Martin Dubslaff[1], Myriano H. Oliveira Jr.[1], Michael Hanke[1], Felix Fromm[2], Thomas Seyller[2,3], J. Marcelo J. Lopes[1], and Henning Riechert[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Lehrstuhl für Technische Physik, Friedrich-Alexander-Universitt Erlangen-Nürnberg, Erlangen, Germany — [3]Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

We report on the synthesis of graphene on a $(6\sqrt{3} \times 6\sqrt{3})$R30° reconstructed SiC(0001) surface (a.k.a. *buffer layer*) by means of molecular beam epitaxy (MBE). Raman spectroscopy reveals that the quality of the MBE-grown graphene films increases with growth time and that the average crystallite size exceeds 20 nm. X-ray photoelectron spectroscopy confirms that the thickness of the films increases as a function of the growth time and proves that the buffer layer is preserved during the growth process. In addition, grazing-incidence X-ray diffraction measurements were performed at the beamline ID10 of the ESRF in Grenoble. In-plane reflections of the buffer layer, the SiC, as well as from the MBE-synthesized graphene, were investigated. Strikingly, despite their nanocrystalline nature, it is observed that the graphene films grown by MBE show an in-plane alignment to the substrate, revealing that a conventional epitaxial growth on the buffer layer takes place. The results will be discussed in the context of MBE growth of graphene considering the most recent data reported in the literature.

O 68.2 Thu 10:45 H17

Microscopic characterization of CVD grown graphene suspended on TEM grids — •Florian Studener[1], Luca Bignardi[1], Willem van. Dorp[1], Steffano Gottardi[1], Oleksii Ivashenko[1], Pavel Dudin[2], Alexei Barinov[2], Petra Rudolf[1], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, Netherlands — [2]Sincrotrone Trieste S.C.p.A, 34149 Basovizza, Trieste, Italy

We investigated CVD grown graphene, which was transferred and suspended on a TEM grid. Both electronic and structural properties were investigated. The former were investigated with angle resolved photoelectron spectroscopy and microscopy, while the latter were analysed with Raman spectroscopy and transmission electron microscopy. We could observe that CVD grown graphene has comparable characteristics with free standing graphene produced with micro cleavage, e. g. the Fermi velocity of 1*10-6 m/s is close to the theoretically expected value. Despite the polycrystalline nature of the Cu foil used as a substrate for the graphene growth, the obtained graphene exhibits large single-crystalline domains up to tens of microns. Thus, the presented transfer method can be successfully exploited for clean TEM substrates for further investigations.

O 68.3 Thu 11:00 H17

Graphene-enhanced versus Surface-enhanced Raman Scattering — •Fatemeh Yaghobian, Tobias Korn, and Christian Schüller — Institute of Experimental and Applied Physics University of Regensburg D-93040 Regensburg, Germany

Graphene-enhanced Raman scattering (GERS) is emerging as an important method due to the need for highly reproducible, quantifiable and biocompatible active substrates. As a result of its unique two dimensional carbon structure, graphene provides particularly large enhanced Raman signals of molecules at its surface. In this work, it is demonstrated that graphene works as active substrate for enhanced Raman scattering and has a great potential in biosensing because of its ability to quench interfering fluorescence. Obtained GERS signals of different molecules with reproducible enhancement factors are discussed and compared with surface-enhanced Raman scattering (SERS) signals on highly active substrates, covered with spherical silver nanoparticles. We have also observed an upshift in the frequency of the breathing mode of a test molecule, when adsorbed on graphene, in contrast to measurements on silver nanoparticles, where the frequencies remain unchanged.

O 68.4 Thu 11:15 H17

Dynamics of adsorbate layers on freestanding graphene probed by ultrafast low-energy electron diffraction — •Max Gulde[1], Simon Schweda[1], Manisankar Maiti[1], Hakki Yu[2], Sascha Schäfer[1], and Claus Ropers[1] — [1]Materials Physics Institute and Courant Research Centre, University of Göttingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, University of Göttingen, Germany

Ultrafast structural dynamics in solids and nanostructures can be observed by an increasing number of sophisticated electron and x-ray diffraction techniques. Despite successful implementations of ultrafast reflection high-energy electron diffraction (1,2), the diffractive probing of ultrafast structural processes at surfaces remains an experimental challenge. We have implemented ultrafast low-energy electron diffraction (ULEED) to study structural changes with high temporal resolution and ultimate surface sensitivity, at electron energies from 100 eV to 500 eV. Specifically, we ultilize nanoscopic needle emitters in an electrostatic lens geometry as high-brightness sources of pulsed electrons. With this approach, the ultrafast melting dynamics of ordered adsorbate structures on freestanding graphene is investigated in transmission with a temporal resolution below 5 ps.

(1) A. Hanisch-Blicharski, A. Janzen, B. Krenzer, S. Wall, F. Klasing, A. Kalus, T. Frigge, M. Kammler, and M. Horn-von Hoegen, Ultramicroscopy (accepted) (2012)

(2) S. Schäfer, W. Liang, and A. H. Zewail, J. Chem. Phys. 135, 214201 (2011)

O 68.5 Thu 11:30 H17

High-Temperature STM of the Ordering of an Amorphous Carbon Layer into Graphene on Ru(0001) — Sebastian Günther[1], Sebastian Dänhardt[2], •Martin Ehrensperger[2], Patrick Zeller[2], Stefan Schmitt[3], and Joost Wintterlin[2] — [1]Chemie Department, Technische Universität München, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, Germany — [3]SPECS GmbH, Voltastr. 5, D-13355 Berlin, Germany

An amorphous carbon layer was prepared on Ru(0001) by chemical vapor deposition of ethylene at about 650 K. High-Temperature Scanning Tunneling Microscopy (HTSTM), Low Energy Electron Diffraction and Temperature Programmed Desorption measurements were used to characterize the layer and its formation. The obtained carbon layer then served as amorphous precursor in an ordering transition towards graphene. At temperatures between 920 and 950 K the layer transformed into graphene which was indicated by the evolving moiré pattern. The ordering was monitored *in situ* by HTSTM. The observations revealed a unique mechanism involving mobile, small topographic holes that move through the disordered carbon layer leaving graphene behind. The transport of carbon monomers mediated by these holes opens a low-energy pathway for the ordering transition. In a dense packed graphene layer this mechanism is impossible which can explain the problems of healing defects in chemically synthesized graphene.

O 68.6 Thu 11:45 H17

***In situ* LEEM Investigations of the Growth of Graphene on Ni(111)-Films** — •Patrick Zeller[1], Michael Weinl[2], Florian Speck[3], Markus Ostler[3], Thomas Seyller[3], Matthias Schreck[2], and Joost Wintterlin[1] — [1]Department Chemie, Ludwig-Maximilians-Universität München — [2]Institut für Physik, Universität Augsburg — [3]Department für Physik, FAU Erlangen-Nürnberg

We report about low energy electron microscopy (LEEM), scanning tunneling microscopy (STM), auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS) investigations of graphene grown on single-crystalline Ni(111) films. The films, which may provide an easy and economical way towards a scalable graphene synthesis, consist of 150 nm thick, heteroepitaxially grown Ni(111) layers on a Si(111) wafer with a YSZ-buffer layer. Monolayer graphene was grown by chemical vapor deposition of ethylene and *in situ* LEEM investigations of the graphene growth were performed. Also the formation of nickel carbide and its transformation into graphene were observed. Furthermore we noticed an involvement of the bulk during the reaction. At the beginning of the ethylene dosing the C atoms dissolve in the bulk, and after nucleation segregation of C atoms starts. We could also observe the healing of rotated graphene towards aligned, high quality graphene in a small temperature range. Also a temperature dependent formation and healing of dislocation lines in the Ni films was observed.

O 68.7 Thu 12:00 H17

Growth of graphene on a stepped iridium surface: morphology, domains and electronic fingerprints — •Iva Šrut[1], Vesna Mikšić Trontl[1], Petar Pervan[1], Fabian Craes[2], Thomas Michely[2], Carsten Busse[2], and Marko Kralj[1] — [1]Institut za fiziku, Bijenička 46, 10000 Zagreb, Croatia — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

A promising route for modification of graphene properties is the growth of graphene on a substrate with a periodic arrangement of steps. We have used scanning tunneling microscopy and spectroscopy (STM/STS) and low energy electron diffraction (LEED) to study the growth of graphene on such periodically stepped Ir(332) surface. We have found that graphene continuously extends over iridium terraces and steps. Moreover, new distinctive mesoscopic features of the underlying surface are formed involving large, flat terraces accompanied by groups of narrower steps [1]. These morphologically different regions are also distinctive by their spectroscopic features found in STS. The distribution of the newly formed terraces as well as the contribution of various graphene orientations is sensitive to the preparation temperature. Below 800°C we find that the terrace width distribution is closer to the intrinsic distribution of clean Ir(332) than for higher temperatures. Additionally, graphene grown at low temperatures has a prominent contribution of a domain rotated by 30° with respect to the substrate. We find that the microscopic shape of steps after graphene formation strongly depends on the orientation of graphene.

[1] I. Šrut, et al., submitted

O 68.8 Thu 12:15 H17

Phonons of graphene on Ir(111) — •Michael Endlich[1], Alejandro Molina-Sánchez[2], Ludger Wirtz[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau — [2]Physics and Material Sciences Research Unit, University of Luxembourg, L-1511 Luxembourg

The phonon dispersion relations of graphene on Ir(111) were determined with angle-resolved inelastic electron scattering. A weak graphene–Ir interaction is inferred from the lifting of the degeneracy of the out-of-plane optical and acoustic dispersion branches at the $\bar{K}$ point of the surface Brillouin zone and from the energy reduction of the out-of-plane optical phonon. Despite this interaction the Kohn anomalies known from graphite of the highest optical phonon branch at $\bar{\Gamma}$ and $\bar{K}$ persist. The experimental dispersion relations are in agreement with density functional calculations.

O 68.9 Thu 12:30 H17

Support restructuring during graphene growth on Cu foils triggers the formation of non flat membranes — •Jürgen Kraus[1], Sebastian Böcklein[2], Robert Reichelt[1], Benito Santos[3], Tevfik O. Mentes[3], Andrea Locatelli[3], and Sebastian Günther[1] — [1]Technische Universität München Chemie Department, D-85748 Garching — [2]Ludwig-Maximilians-Universität, D-81377 München — [3]Sincrotrone Trieste, I-34149 Trieste - Basovizza

Meanwhile the growth of single crystalline graphene flakes on Cu foils at a mm-length scale can be achieved, which provides a potential source for high quality graphene. On the other hand, the g-Cu system still suffers from certain inherent defects: during graphene growth sequences of inclined Cu facets form which are visible in scanning electron microscopy (SEM) images as stripes and which have been observed as well applying atomic force microscopy (AFM) and scanning tunneling microscopy (STM). Since the graphene follows the morphology of the underlying Cu foil the support restructuring leads to the formation of so called nanorippled graphene which persists even if the graphene is transferred on a flat Si wafer. In our study, we identified a sequence of such Cu facets after graphene growth on a Cu foil using low energy electron microscopy (LEEM) and show why the graphene cannot flatten when removed from the support. In addition, we were able to prepare graphene membranes by the local electrochemical removal of the Cu foil underneath the grown graphene. We show that the resulting membranes are exact replicas of the former morphology of the Cu foil during growth, i.e. they are non flat membranes.

O 68.10 Thu 12:45 H17

Graphene on Rh(111) and Ru(0001): combined STM/NC-AFM and DFT studies — •Yuriy Dedkov[1], Torben Haenke[1], Oliver Schaff[1], Andreas Thissen[1], Elena Voloshina[2], and Mikhail Fonin[3] — [1]SPECS Surface Nano Analysis GmbH, Voltastraße 5, 13355 Berlin, Germany — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [3]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The electronic and crystallographic structure of graphene moiré on Rh(111) and Ru(0001) is studied via combination of density-functional theory calculations and scanning tunneling and noncontact atomic force microscopy (STM and NC-AFM). Whereas the principal contrast between hills and valleys observed in STM does not depend on the sign of applied bias voltage, the contrast in atomically resolved AFM images strongly depends on the frequency shift of the oscillating AFM tip. The obtained results demonstrate the perspectives of application atomic force microscopy/spectroscopy for the probing of the chemical contrast at the surface.

O 68.11 Thu 13:00 H17

Epitaxial graphene nanoflakes on Au(111): Structure, electronic properties and manipulation — •Mikhail Fonin[1], Philipp Leicht[1], Lukas Zielke[1], Elena Voloshina[2], and Yuriy

S. Dedkov[3] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [3]SPECS Surface Nano Analysis GmbH, 13355 Berlin, Germany

Graphene nanoribbons and graphene dots have been proposed to exhibit such peculiar phenomena like localized edge states or edge magnetism. The aim of the present study is the investigation of structural and electronic properties of epitaxial graphene nanoflakes on the Au(111) surface.

Upon in situ preparation, we observe a formation of two types of nanoflakes, which are either embedded in the gold surface or sit directly on top of Au(111). In all cases, flakes reveal a moiré contrast, which is modulated by the herring-bone reconstruction of the Au(111) surface with the moiré period depending on the orientation of the graphene sheet in relation to the substrate. We show that quasi-free-standing graphene nanoflakes can be easily manipulated by the STM tip regardless of the flake size. The details of the structure and electronic properites of such quasi-free-standing flakes are discussed upon comparison with graphene dots on Ir(111).

O 69: Invited Talk (Marc Koper)

Time: Thursday 15:00–15:45 Location: H36

Invited Talk O 69.1 Thu 15:00 H36
Electrocatalysis: from single crystals to single nanoparticles — •Marc Koper — Leiden Institute of Chemistry, Leiden University, the Netherlands

The surface science approach to electrocatalysis is very useful in understanding the structure sensitivity effect for a number of well-known electrocatalytic redox reactions. We show here that the important distinction of two types of surface sensitivity: reactions that prefer defects in (111) facets, typically those involving O-H and C-H bond making and breaking, and reactions that prefer (100) terraces, typically those involving C-C, C-O, N-N, and N-O bond making and breaking. This has automatic implications for nanoparticle design. Finally, we will show how the measurement of electrocatalysis at single nanoparticles can be performed, including the associated complications.

O 70: Symposium Photons in Magnetism (SYPM, jointly with MA, HL, MI)

Time: Thursday 15:00–17:30 Location: H1

Invited Talk O 70.1 Thu 15:00 H1
Ultrafast emergence of nanoscale ferromagnetism far from equilibrium — •Hermann Dürr — SLAC National Accelerator Laboratory, Menlo Park USA

Long-range magnetic order in solids is usually ascribed to the exchange interaction between electron spins. Close to equilibrium this leads to spontaneous magnetization when the system cools below the magnetic ordering temperature. We show that the far from equilibrium flow of angular momentum via spin currents can also achieve long-range ferromagnetic order even above the ordering temperature. To reveal this process, we use ultrafast x-ray diffraction at SLAC's Linac Coherent Light Source to probe the nucleation, growth and transient existence of ferromagnetic order on the nm length and fs timescale after fs optical laser excitation has brought a metallic 3d - 4f alloy system into a highly non-equilibrium chaotic spin state. The technological exploitation of this effect could pave the way for novel ways to manipulate and transport information within the smallest space-time dimensions.

Invited Talk O 70.2 Thu 15:30 H1
Free-Electron Laser for Ultrafast Measurements in Material Science — •Sven Reiche — Paul Scherrer Institute, Villigen, Switzerland

Free-electron Lasers provide intense and coherent photon pulses with femtosecond pulse duration down to the Angstron wavelength level. With ability to freely adjust the resonant wavelength and polarization it became a unique instrument to study ultrafast process on the Atomic level in a broad range of research fields. This presentation gives a brief introduction on the functionality of a Free-electron LAser and possible application for material science.

Invited Talk O 70.3 Thu 16:00 H1
Nanomagnetism seen by Femtosecond X-rays — •Stefan Eisebitt — Institut für Optik und Atomare Physik, Technische Universität Berlin

Magnetism exhibits phenomena on intrinsic timescales spanning many orders of magnitude. Femtosecond light sources have given us access to ultrafast de/remagnetization phenomena. Due to their short wavelength, novel fs X-ray sources allow us to probe such phenomena in conjunction with spatial information at the nanoscale. I will report on resonant scattering experiments at Free Electron X-ray Lasers, which allow us to observe the influence of electronic transport in the presence of magnetic domains on ultrafast demagnetization phenomena. In addition, ultrafast real space observation of magnetic domains via x-ray holography using single fs-pulses from X-ray lasers has become a reality and will be discussed.

Invited Talk O 70.4 Thu 16:30 H1
Ultrashort Radiation Pulses at Storage Rings — •Holger Huck — Zentrum für Synchrotronstrahlung, Technische Universität Dortmund, Deutschland

With the advent of linac-based SASE-FELs, the investigation of ultrashort phenomena on the sub-picosecond scale is becoming a rapidly growing field of research. Synchrotron radiation sources based on storage rings offer a broad range of photon energies and higher repetition rates than linear accelerators, but have an inherently longer pulse duration of typically several ten picoseconds. However, different techniques have been developed to generate ultrashort radiation pulses ranging from the THz to the X-ray regime at storage rings. Several of these techniques will be outlined in this talk. For example in Germany, BESSY, ANKA and the MLS are regularly operated in low-alpha mode, a femto-slicing source exists at BESSY, and the CHG (coherent harmonic generation) scheme is employed by the DELTA short-pulse facility, for which EEHG (echo-enabled harmonic generation) is planned as an upgrade.

Invited Talk O 70.5 Thu 17:00 H1
Every atom counts - Magnetic properties of supported metal atoms and small alloy clusters — Torben Beeck, Ivan Baev, Steffen Palutke, Kai Chen, Sören Meyer, Kari Jänkälä, Michael Martins, and •Wilfried Wurth — Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg

Investigation of supported metal atoms and small clusters with a well-defined number of atoms gives fundamental insights into the evolution of magnetic properties from single atoms to nanostructures. Experimental results can be compared to theoretical studies since the supported small clusters present tractable systems for sophisticated theoretical methods that explicitly include strong correlation effects. Experimentally the magnetic properties can be investigated using magnetic circular dichroism in resonant x-ray absorption (XMCD). XMCD at modern synchrotron radiation sources such as BESSY II in Berlin and PETRA III in Hamburg allows us - due to its element specificity - to investigate very dilute targets such as small particles with very few atoms even on a large background, i.e. in contact with a metal substrate. In the talk I will review results on single metal atoms as well as small alloy clusters with a defined number of atoms and composition in contact with a metal substrate which illustrate how the local properties such as spin and orbital magnetic moment strongly depend on the interaction within the cluster and with the substrate.

Support by the DFG through SFB 668 and by the BMBF through grant 05K10GU5 is gratefully acknowledged.

O 71: Surface Magnetism (jointly with MA)

Time: Thursday 15:00–18:45 Location: H3

Invited Talk O 71.1 Thu 15:00 H3

Spin-polarized scanning field emission microscopy and spectroscopy — •Anika Schlenhoff — Institute of Applied Physics, University of Hamburg

High electric fields can discharge electrons from a solid, thereby generating an emission current, which becomes spin-polarized when using a magnetic emitter. A very local injection of these electrons is achieved when approaching a magnetic tip to a sample in an SP-STM setup, and scanning allows for magnetic imaging by means of spin-polarized emission conductivity measurements. Although field emission is routinely used for microscopy purposes, the question remained open how it affects magnetism on the local scale. A detailed understanding of the interplay of hot-electron spins with magnets is essential for the interpretation of many hot electron spin phenomena and characterization techniques, as well as for applications in spintronic devices.

Here we show that a spin-polarized field-emission current resonantly injected into magnets, consisting of only about 50 iron atoms on a W(110) surface, generates considerable Joule heating and spin-transfer torque, thereby severely affecting the thermally driven magnetization reversal. The switching frequency is increased due to phonon generation, and a lifetime asymmetry develops with increasing emission current, most likely driven by Stoner excitations. Even magnetization reversal of quasistable nanomagnets can be triggered by spin-polarized field-emission. Our experiments demonstrate the capability of spin-polarized scanning field emission microscopy for magnetic observation and controlled manipulation on the atomic scale at nm distances.

O 71.2 Thu 15:30 H3

Large wave vector surface spin waves of the nanomartensitic phase in ultrathin iron films on Cu(100) and fcc Co(100) — •Rajeswari Jayaraman, Harald Ibach, and Claus M. Schneider — Peter Grünberg Insitut, Forschungszentrum Jülich, 52425 Jülich, Germany

It is generally accepted that thin-film magnetism is strongly affected by even small structural modifications. Much less is known about the influence of structure on magnetic excitations, in particular, spin waves. Using electron energy loss spectroscopy we have studied the dispersion of large wave vector surface spin waves of a system for which details of the structure became known only recently, namely ultrathin iron films grown on Cu(100) surfaces. We find the spin wave dispersion to be nearly identical to the dispersion reported for bcc Fe(110) layers grown on W(110). We therefore conclude that the spin wave signal stems from the "nanomartensitic" phase of Fe/Cu(100) and that this phase is not merely a surface phase but encompasses the deeper layers. The same spin wave dispersion and LEED pattern as for the Fe/Cu(100) system is observed when Fe is deposited on fcc Co(100)/Cu(100). We therefore conclude that these Fe films likewise assume the nanomartensite structure.

O 71.3 Thu 15:45 H3

Parity effect in ground state localization of antiferromagnetic chains coupled to a ferromagnet — Simon Holzberger[1], Tobias Schuh[1], Samir Lounis[2], Stefan Blügel[2], and •Wulf Wulfhekel[1] — [1]Physikalisches Institut, KIT — [2]Peter Grünberg Institut, Forschungszentrum Jülich

We investigate the ground states of antiferromagnetic Mn nanochains on Ni(110) by spin-polarized scanning tunneling microscopy in combination with theory. While the ferrimagnetic linear trimer experimentally shows the predicted collinear classical ground state, no magnetic contrast was observed for dimers and tetramers where non-collinear structures were expected based on ab-initio theory. This striking observation can be explained by zero-point energy motion for even numbered chains derived within a classical equation of motion leading to non classical ground states. Thus, depending on the parity of the chain length, the system shows a classical or a quantum behavior.

O 71.4 Thu 16:00 H3

Constant current contrast in spin-polarized STM — •Krisztian Palotas — Budapest University of Technology and Economics, Department of Theoretical Physics, Budapest, Hungary

This work is concerned with the theoretical description of the contrast, i.e., the apparent height difference between two lateral surface positions on constant current spin-polarized scanning tunneling microscopy (SP-STM) images.

We propose a method [1] to predict the bias voltage dependent magnetic contrast from single point tunneling current or differential conductance measurements, without the need of scanning large areas of the surface. Depending on the number of single point measurements, the bias positions of magnetic contrast reversals and of the maximally achievable magnetic contrast can be determined. We validate this proposal by simulating SP-STM images on a complex magnetic surface employing a recently developed approach based on atomic superposition [2]. Furthermore, we show evidence that the tip electronic structure and magnetic orientation have a major effect on the magnetic contrast. Our theoretical prediction should inspire experimentalists to considerably reduce measurement efforts for determining the bias dependent magnetic contrast on magnetic surfaces.

This research was supported by the OTKA PD83353, K77771, TAMOP-4.2.2.B-10/1-2010-0009 projects, and a Bolyai Grant.

[1] K. Palotas, arXiv:1207.3995 (2012).

[2] K. Palotas et al., Phys. Rev. B 83, 214410 (2011); Phys. Rev. B 84, 174428 (2011); Phys. Rev. B 85, 205427 (2012).

O 71.5 Thu 16:15 H3

Mapping the energy landscape of the magnetoelectric phase transition in Fe nanoislands — •Lukas Gerhard[1], Rien Wesselink[1,2], Arthur Ernst[3], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, 7500AE Enschede, The Netherlands — [3]Max-Planck-Institut fuer Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

Magnetoelectric coupling (MEC) offers the possibility to control the magnetic state of a material by applying an electric field raising the prospect of new applications in magnetic storage devices. Using the electric field of a scanning tunneling microscope (STM) tip we recently demonstrated strong MEC in metallic nano islands [1]. High electric fields of the order of 1 GV/m trigger a crystallographic and magnetic phase transition from antiferromagnetic fcc to ferromagnetic bcc in bilayer Fe islands on a Cu(111) surface. An extensive statistical analysis of the thermally activated switching at subcritical electric fields unveils the characteristic energies of the balance between the two states. We map this energy landscape as function of strain and electric field which gives us a thorough understanding of the critical parameters necessary to fine-tune the dynamics of MEC induced phase transitions. [1] L. Gerhard et al. Magnetoelectric coupling at metal surfaces. Nat. Nano 5, 792-797 (2010)

O 71.6 Thu 16:30 H3

Role of magnetism in Catalysis: RuO2 (110) surface — •Engin Torun[1], Changming Fang[1,3], Gilles A de Wijs[1], and Robert de Groot[1,2] — [1]Electronic Structure of Materials, Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [2]Laboratory of Chemical Physics, Zernike Institute of Advanced Materials, Nijenborgh 4, NL-9747 AG Groningen, The Netherlands — [3]University of Vienna, Faculty of Physics, Computational Materials Physics, Sensengasse 8/12, 1090 Wien, Austria

The three conservation laws (energy, momentum and angular momentum) are well known, but the consequences of the last one are too often neglected. A clear example in electrochemistry is the electrolysis of water. Hydrogen production by electrolysis of water seemingly violates conservation of angular momentum because only one magnetic species is involved (oxygen). The losses in electrolysis are overwhelmingly dominated by the production of oxygen. While the ground state of oxygen is magnetic its first and second excited states are non-magnetic singlet states. This explains the losses at the anode. The oxygen is initially produced in a non-magnetic excited state. A fundamental solution of this problem is only possible by the introduction of a second magnetic species. We report calculations on the surface electronic structure of one of the best anodes, the RuO2 (110) surface. This surface itself is magnetic and a mechanism will be proposed how this second magnetic species allows the production of oxygen in its magnetic ground state. A similar situation in biology will be discussed.

O 71.7 Thu 16:45 H3

Scanning tunneling spectroscopy of quantum well states in thin Pd(001) films — •Sujit Manna[1], Marek Przybylski[1,2], and Jürgen Kirschner[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Kraków, Poland — [3]Naturwissenschaftliche Fakultät II, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Scanning Tunneling Spectroscopy (STS) on transition metals with filled d-bands below Fermi level is hardly expected to yield features due to the d-states because their contribution to the tunneling current is much smaller than that of the sp-band states. We have investigated the electronic structure of thin Pd films grown on Cu(001) by STS at T=4.7K with single layer thickness resolution. We have identified the occupied d-band quantum well states (QWS), which arise from the electron confinement along the growth axis of Pd films and give rise to sharp peaks in the tunneling spectra. A quantitative analysis of the spectra yields the band dispersion, which is similar to the calculated free electron dispersion in bulk Pd along the Γ-L direction. Also the correlation between the QWS formed in the Pd films with magnetic anisotropy (MA) of adjacent Co films in the Co/Pd bilayer system will be shown and discussed. The step induced uniaxial MA is found to oscillate as a function of Pd film thickness with a period of 6 ML, in agreement with theoretical calculations [1]. [1] M. Cinal, J. Phys.: Condens. Matter 13, 901 (2001).

15 min. break

O 71.8 Thu 17:15 H3

Spin-dependent Smoluchowski effect — •Marco Corbetta[1], Oleg Polyakov[1,2], Oleg Stepanyuk[1,2], Hirofumi Oka[1], Aleksander Saletsky[2], Dirk Sander[1], Valeriy Stepanyuk[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [2]Faculty of Physics, Moscow State University, Moscow, Russia

The Smoluchowski effect [1] focuses on the total electron charge density and it neglects that electrons carry a spin. In spin-polarized materials, it is not clear how majority and minority states contribute to the spin-dependence of this effect. To elucidate this point we perform spin-polarized scanning tunneling microscopy at the step edge of a bilayer high Co island on Cu(111) at 8 K. We measure maps of the differential conductance (dI/dV) for states of parallel (P) and anti-parallel (AP) orientation between tip and sample magnetization. From these maps we extract the asymmetry A of the differential conductance A=(dI/dVAP-dI/dVP)/(dI/dVAP+dI/dVP). This quantity is proportional to the spin polarization of the sample. We reveal striking spatial variations of the spin-polarization at the transition between the Co step and the Cu substrate with sub-nm spatial resolution and investigate its energy dependence. We find a variation of the tunnel magneto resistance ratio of more than 20% on a length scale of few Angstroms. We discuss our results on the basis of ab-initio calculations, spin-dependent electron charge flow supports our findings [2]. [1] R. Smoluchowski, Phys. Rev. 60, 661 (1941). [2] O. P. Polyakov et al., Phys. Rev. B, accepted (2012).

O 71.9 Thu 17:30 H3

Temperature-dependent magnetic hysteresis of the differential conductance in spin-polarized scanning tunneling spectroscopy with Fe-coated W tips — •Soo-hyon Phark[1], Jeison Fischer[1,2], Marco Corbetta[1], Dirk Sander[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Laboratório de Filmes Finos e Superfícies, Departamento de Física, Universidade Federal de Santa Catarina , Florianópolis, SC, Brazil

We performed spin-polarized scanning tunneling spectroscopy on bilayer high Co islands of the nm size range [1] on Cu(111) for temperatures between 10 and 30 K in magnetic fields oriented normal to the sample surface. We use a W tip, heated to 2200 K in UHV, coated with 40-monolayer Fe. Increasing the temperature from 10 to 30 K, we observe a decline of the switching field of an individual Co island, and a reduced slope of the differential conductance around zero field [2]. The Néel-Brown model for the magnetic reversal process of the Co islands and a superparamagnetic response of the tip magnetization as described by the Langevin function gives a favorable description of the data. We estimate that the tip apex is composed of roughly 200 Fe atoms. This suggests that a Fe cluster, rather than a Fe film, determines that magnetic response of the tip. The role of the magnetic stray field of the Co island for the magnetic response of the tip is discussed.

[1] Ouazi, Wedekind, Rodary, Oka, Sander, Kirschner, Phys. Rev. Lett. 108, 107206 (2012). [2] Rodary, Wedekind, Sander, Kirschner, Jap. J. Appl. Phys. 47, 9013 (2008).

O 71.10 Thu 17:45 H3

Magnetic coupling of single Co adatoms through Pd spacer layers — •Liudmila Dzemiantsova, Mahboubeh Hortamani, Christian Hanneken, André Kubetzka, Kirsten von Bergmann, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg, Germany

The knowledge about the magnetic coupling on the atomic scale is crucial for the tailoring magnetic devices in reduced dimensions and the tuning their properties [1]. In particular, the dependence of the exchange coupling of magnetic adatoms on the thickness of the spacer layer is important for the fundamental understanding of magnetism and practical applications in spin-based technology [2].

We performed a combined experimental and theoretical investigation of Co atoms on top of a Pd spacer on Co/Ir(111). Using spin-polarized STM, spin contrast is achieved on Pd mono (ML)- and double-layer (DL) and on Co adatoms, which means that the electron density above the surfaces and adatoms is spin-polarized. In accordance with our experimental observations of Co atoms on the Pd spacer, our *ab initio* calculations show that Co layers adsorbed on top of a Pd mono- and double-layer are ferromagnetically coupled to the Co/Ir(111) underneath. The size of the magnetic coupling is reduced by a factor of three from a ML to a DL Pd spacer between the Co layers [3].

[1] F. Meier *et al.*, Science, 320, 82 (2008).
[2] A. A. Khajetoorians *et al.*, Science, 332, 1062 (2011).
[3] L. V. Dzemiantsova *et al.*, Phys. Rev. B, 86, 094427 (2012).

O 71.11 Thu 18:00 H3

Complex Magnetism in Fe nanoclusters on Ir(111) — •David Bauer, Phivos Mavropoulos, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

Recently, a square lattice of skyrmions of nanoscale dimension has been experimentally identified by spin-polarized scanning tunneling microscopy combined with first-principles calculations [1] as the magnetic ground state of an hexagonal Fe monolayer on the Ir(111) substrate. The magnetic structure is a result of a fine balance between the Heisenberg and biquadratic exchange, the four-spin interaction, magnetic anisotropy and the Dzyaloshinskii-Moriya interaction. This raises the question whether a single skyrmion is already encoded in a minimal hexagonal cluster of 7 atoms or *e.g.* in the next larger one of 19 atoms. To shed light onto this problem we apply our recently developed all-electron full-potential relativistic Korringa-Kohn-Rostoker Green-function method jointly with a model spin-dynamics code to study the non-collinear magnetism in finite nano-structures and clusters perfectly embedded in bulk materials or on surfaces.We find that the finite size of these clusters changes the balance between the magnetic interactions significa ntly. For example, also for the 19 atom cluster a strong non-collinear formation of spins was found, but qualitatively different to the skyrmion in the sense that most spins relax to an almost rectangular alignment with respect to their neighbors indicating that the Dzyaloshinskii-Moriya interaction determines the magnetic structure.

[1] S. Heinze et al. Nature Phys. **7**, 713 (2011).

O 71.12 Thu 18:15 H3

Nano-skyrmions lattices and magnetic phase diagram of Fe/Ir(111) — •Nikolai Kiselev, David Bauer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, a square lattice of skyrmions of nanoscale dimension has been experimentally identified by spin-polarized scanning tunneling microscopy combined with first-principle calculations [1] as the ground state of an hexagonal Fe monolayer on the Ir(111) substrate. Here, we present a detailed theoretical description of the magnetic phase diagram of Fe/Ir(111) obtained from Monte Carlo simulations in extended Heisenberg model employing parameters obtained from first-principles calculations. We give a comprehensive analysis of the ground state and field/temperature induced transitions and compare our results with experiment. We predict the existence of a new modulated state: an hexagonal lattice of skyrmions stabilized at high field and temperature. The transition between hexagonal and square skyrmion lattices is characterized by an extremely strong hysteretic effect and the abrupt change of the topological number. We discuss in details general aspects of the nano-skyrmions, in particular leading terms in the Hamiltonian, which are responsible for the stability of skyrmions in low dimensional magnetic systems.

[1] S. Heinze et al. Nature Phys. 7, 713 (2011).

O 71.13 Thu 18:30 H3

Ab initio study of ferromagnetic Co-chains on the (5x1) Iridium(001) surface — •Bertrand Dupe[1], Yuriy Mokrousov[2], and Stefan Heinze[1] — [1]Institut für Theoretische Physik und Astrophysik, CAU Kiel, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation Forchungszentrum Jülich,Jülich, Germany

Nanostructures of 3d transition metals on 4d or 5d substrates have been shown to exhibit complex spin structures [1-4]. A recent study demonstrated the intriguing magnetism of Fe biatomic chains on the (5x1) reconstructed Ir(001) surface due to the interplay of magnetocrystalline anisotropy, Dzyaloshinskii-Moriya interaction and exchange interaction [4]. Here, we use first-principles calculations based on density functional theory to explore Co biatomic chains on the (5x1) Ir(001) surface. Due to the key role of 3d-5d hybridization for the magnetic properties of such systems [5], we study Co chains in different structural arrangements and the impact of structural relaxations. We report the magnetic properties of the Co chains such as the magnetocrystalline anisotropy energy and the spatial distribution of spin-polarization. We compare our results with recent spin-polarized STM experiments [6].

[1] B. Hardrat et al. PRB 79, 094411 (2009) [2] S. Heinze et al. Nature Phys. 7, 713 (2011) [3] Y. Yoshida et al., PRL 108, 087205 (2012) [4] M. Menzel et al PRL, 108, 197204 (2012) [5] S. Baud et al Phys. Rev. B 73, 104427 (2006) [6] J. Bickel, K. et al to be published

O 72: Graphene: Theory (jointly with DS, HL, MA, and TT)

Time: Thursday 15:00–17:30 Location: H17

O 72.1 Thu 15:00 H17

Influence of non-local exchange-correlation and spin-orbit interaction on electronic and optical properties of graphene, silicene, germanene, and tinene — •Lars Matthes[1], Olivia Pulci[2], Paola Gori[3], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Dipartimento di Fisica, Università di Roma "Tor Vergata", via della Ricerca Scientifica 1, 00133 Rome, Italy — [3]CNR-ISM, Via Fosso del Cavaliere 100, 00133 Rome, Italy

We present first-principles studies of the optical absorbance of the group-IV honeycomb crystals graphene, silicene, germanene, and tinene. We account for many-body effects on the optical properties by using the non-local hybrid functional HSE06. The optical absorption peaks are blue-shifted due to quasi-particle corrections, while the influence on the low-frequency absorbance remains unchanged and reduces to the universal value $\pi\alpha$,[1,2] where α is the Sommerfeld fine-structure constant. However, in silicene, germanene and tinene an electronic band gap arises at the Dirac-point due to spin-orbit splitting and parabolic bands with a very small effective mass emerge. Consequently, the low-frequency absorbance is modified due to the spin-orbit induced fundamental absorption edge. We demonstrate numerically that the absorbance increases at the fundamental absorption edge.

[1] A. Geim et al., Science 320, 1308 (2008)

[2] F. Bechstedt, L. Matthes et al., Appl. Phys. Lett. 100, 261906 (2012)

O 72.2 Thu 15:15 H17

Generalized Hubbard models for two dimensional hybrid materials — •M. Rösner[1], E. Sasioglu[2], C. Friedrich[2], S. Blügel[2], A. I. Lichtenstein[3], M. I. Katsnelson[4], and T. O. Wehling[1] — [1]Institut für Theoretische Physik, Universität Bremen, D-28359 Bremen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]1. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [4]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands

We present effective generalized Hubbard models for the description of novel two dimensional materials. The local and non-local partially screened Coulomb interaction as well as hopping integrals are calculated from first principles for silicene and graphene on a metallic substrate. We consider interactions up to the 6th nearest neighbor in real space and investigate the long range behavior of the dielectric function in k-space. We compare the resulting silicene Hubbard model to the corresponding model for pure graphene. Thereby we find values of $U/t \approx 4.0$ eV for the on-site and $V/t \approx 2.4$ eV for the nearest neighbor partially screened Coulomb interaction in silicene, which are slightly bigger than in freestanding graphene. We further show that the ratio of the local to the non-local Coulomb interaction can be controlled by a metallic substrate, which efficiently screens non-local Coulomb terms.

O 72.3 Thu 15:30 H17

Subgap conductivity in gated bilayer graphene — •Maxim Trushin — University of Konstanz, 78457 Konstanz

In the present work [1], the subgap electron transport has been investigated in gated bilayer graphene [2] within the two-band effective model using the finite-size Kubo formula. The conductivity does not vanish even though the temperature is set to zero and the chemical potential gets into the middle of the band gap. In contrast to the universal subgap conductivity observed in the 2D topological insulators [3], the subgap conductivity in bilayer graphene turns out to be sensitive to the band gap size and disorder strength.

The effect can be explained in terms of the quantum mechanical interband coherence which turns out to be important for the chiral carriers. At finite temperature, a competition between the temperature-dependent interband decoherence and thermal activation processes results in the non-monotonic conductivity vs. temperature dependence. The non-monotonicity can be seen as a signature of the interband entanglement responsible for the difference between the transport and spectral gaps. The effect can be observed in gapped bilayer graphene sandwiched in boron nitride where the electron-hole puddles and flexural phonons are strongly suppressed.

[1] M. Trushin, Europhys. Lett. **98**, 47007 (2012). [2] E. McCann, Phys. Rev. B **74**, 161403 (2006). [3] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).

O 72.4 Thu 15:45 H17

Lattice dynamics of few-layer graphene after ultrashort laser excitation — •Naira Grigoryan, Eeuwe S. Zijlstra, and Martin E. Garcia — Universität Kassel, Kassel, Germany

Femtosecond laser pulses may induce striking structural effects in solids via electronic excitation. Here we studied the phonon dynamics on the 10 ps timescale in thin graphite films as a function of its thickness after laser interaction using ab initio molecular dynamics simulations including a Van der Waals force correction term to the local density approximation. We implemented the coupling of the hot electrons with the so-called strongly coupled optical phonons (SCOPs) [T. Kampfrath et al., PRL 95, 187403 (2005)] in a semiempirical way . From our simulations we could determine the decay of the SCOPs into other phonon modes, in particular, the out-of-plane lattice vibrations.

O 72.5 Thu 16:00 H17

RKKY Interaction in a Graphene Bilayer — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

RKKY interaction in doped graphene monolayer ($k_F \neq 0$) shows Friedel oscillations decaying as $1/r^2$ [1]. In this work we consider the RKKY interaction in AA- and AB-stacked bilayer graphene using exact low energy Green's functions. Apart from the common site-to-site interaction we discuss impurities located at the bond centers as well as impurities at the center of the hexagonal plaquettes and intercalant-type impurities located in-between the two carbon layers. Similarly to the monolayer case, we find an oscillatory $1/r^2$ decay for on-site impurities in AA-stacked bilayer graphene. The exchange integral separates

into the product of an energy dependent oscillation and an additional modulation resulting from the interlayer coupling. Interestingly, for on-site impurities in AB-stacked bilayer graphene this additional modulation vanishes at low Fermi energies. Moreover, due to the interference of the neighboring site-to-site interactions, at high Fermi energies the RKKY interaction between two plaquette impurities shows a $1/r^3$ behavior.
[1] M. Sherafati and S. Satpathy, Phys. Rev. B 84, 125416, 2011

Coffee break

O 72.6 Thu 16:30 H17

***Ab initio* calculations of functionalized graphene nanoribbons** — •Christian Till, Nils Rosenkranz, Christian Thomsen, and Janina Maultzsch — TU Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, 10623 Berlin

Since nearly 30 years the discovery and subsequent research on fullerenes, carbon nanotubes, and graphene fuel expectations on carbon-based nanoelectronics. In this context, thin stripes of the two-dimensional material graphene, so-called graphene nanoribbons (GNRs), draw broad interest as well. In this work, we present a comprehensive ab initio study of the structural, electronic and vibrational characteristics of a 7-armchair GNR with hydroxyl functionalized edges. Our results show AGNRs with increasing hydroxyl saturation to be particularly stable. In addition, we find a variation of the ribbon geometry under functionalization. An increasing degree of functionalization leads to a compression perpendicular to the ribbon axis. As a consequence we find a linear shift of the band gap with growing edge hydroxylation. With regard to a possible experimental determination of the degree of functionalization, we indicate fingerprint vibrational modes of the hydroxyl groups as well as a substantial shift of Raman active phonons.

N. Rosenkranz, C. Till, C. Thomsen, and J. Maultzsch, Phys. Rev. B **84**, 195438 (2011).

O 72.7 Thu 16:45 H17

Phonon dispersions of AB- and ABC-stacked graphene trilayers and multilayers — •Bart Verberck[1,2], Karl H. Michel[1], and Björn Trauzettel[2] — [1]Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Recently, it was experimentally confirmed that the electronic structure of graphene multilayers crucially depends on how they are stacked. The simplest multilayer for which different stackings can be realised is the trilayer. The ABA variant features both linearly and quadratically dispersed electronic bands near the K-point, while the ABC variant has cubic electronic dispersion. At the same time, the difference between the phonon dispersions for ABA and ABC trilayer graphene is less well established. Detailed knowledge of the phonon spectra is, however, essential for understanding double-resonant Raman scattering experiments, offering a simple means for characterising multilayer graphene samples (number of layers and stacking sequence). Here we present a theoretical study of the phonon dispersions of AB- and ABC-stacked multilayers based on a phenomenological force-constants model. We find that the difference between the phonon spectra for the two variants is much less apparent than the difference between the respective electronic band structures; the main distinction concerns the low-energy phonon modes around the K-point. We argue that the observed difference in double-resonant Raman scattering signals for ABA and ABC trilayers mainly originates from the different electronic dispersions.

O 72.8 Thu 17:00 H17

Optical selection rules in graphene quantum dots — •Eleftheria Kavousanaki and Keshav Dani — Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology, Graduate University, Okinawa, Japan

We theoretically study the optical absorption of graphene quantum dots for different shapes, sizes and edge types. We calculate the single particle energy spectrum using the tight-binding Hamiltonian and the Dirac-Weyl equation and show that dots with zigzag edges exhibit a degenerate shell of zero energy states, in agreement with previous results. Using standard group theoretical tools, we identify the optical selection rules for triangular and hexagonal quantum dots and discuss the role of light polarization on the absorption spectrum. Finally, we calculate the oscillator strengths and absorption spectra for different quantum dot sizes and identify the contribution of the zero energy states therein.

O 72.9 Thu 17:15 H17

Electronic reflection for a single layer graphene quantum well — •Abir Mhamdi[1,2], Emna Ben Salem[1], and Sihem Jaziri[3] — [1]Laboratoire de Physique de la Matière Condensée, Faculté des Sciences de Tunis, Tunisia — [2]Institut für Theoretische Physik, Georg-August Universität Göttingen, Germany — [3]Laboratoire de Physique des Matériaux, Faculté des Sciences de Bizerte, Tunisia

We address the problem of Dirac fermions' graphene quantum well (GQW) and we focus on the low energy approximation for the Hamiltonian of the system where the former can be described by a Dirac-like Hamiltonian. Interesting relations are obtained and used to discuss the influence of the spin-orbit coupling, which induces an effective mass-like term, on the transport properties of single-layer graphene quantum well. It is found that the reflection probability of incident electrons is sensitive to the effective mass-like term. This can be explained by the dependence of reflection coefficient R on the incident electrons' direction and their energies. Notably, we found that the reflection probability for massive fermions with a very small angle, i.e. the wave-vector along the transport direction is zero in the GQW, can be greatly suppressed.

O 73: Organic Electronics and Photovoltaics II (jointly with CPP, DS, and HL)

Time: Thursday 15:00–18:45 Location: H34

Invited Talk O 73.1 Thu 15:00 H34

Quantum coherence controls the charge separation in a prototypical artificial light harvesting system — •C. Lienau[1], S. M. Falke[1], C. A. Rozzi[2], N. Spallanzani[2], A. Rubio[2], E. Molinari[2], D. Brida[3], M. Maiuri[3], G. Cerullo[3], H. Schramm[4], and J. Christoffers[4] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]Istituto Nanoscienze - CNR, Centro S3, Modena, Italy — [3]IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Italy — [4]Institut für Reine und Angewandte Chemie, Carl von Ossietzky Universität Oldenburg, Germany

The efficient conversion of light into electricity or chemical fuels is a fundamental challenge. In artificial photosynthetic and photovoltaic devices this conversion is generally thought to happen on ultrafast time scales in the fs to ps range and to involve an incoherent electron transfer process. In some natural biological systems, however, there is now growing evidence that the coherent motion of electronic wavepackets is an essential primary step, raising questions about the role of quantum coherence in artificial devices. Here we investigate the primary charge transfer process in a supramolecular triad, a prototypical artificial reaction center. Combining high time-resolution femtosecond spectroscopy and time-dependent density functional theory, we provide compelling evidence that the driving mechanism of the photoinduced current generation cycle is a correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds. We highlight the fundamental role of the interface between chromophore and charge acceptor in triggering the coherent wavelike electron-hole splitting.

O 73.2 Thu 15:30 H34

Simulations of Electron Transfer in a Fullerene Hexa-Pyropheophorbide-a Complex — •Thomas Plehn, Jörg Megow, and Volkhard May — Humboldt-Universität zu Berlin, Germany

Electron transfer (ET) is studied between electronically excited chromophores and a C60 fullerene forming a highly flexible complex, which is dissolved in a solvent. Such investigations are of particular interest with regard to future artificial photosynthetic reaction centers and respective applications in future components of photovoltaic devices. The whole discussion is based on extended MD-simulations. To obtain reliable ET results three differently advanced theories are used. The first treatment uses the classical Marcus theory. Respective Marcus parameters are obtained from literature [1]. A generalized ansatz can be derived by the Landau-Zener theory [2]. Secondly, a semi-classical surface-hopping method [3] is chosen. For this approach the conformation-dependent free-energy surfaces and Marcus parameters are calculated directly from the MD-trajectory. The third approach uses the dispersed-polaron/spin-boson model [3]. This method enables the approximation of a quantum-mechanical harmonic oscillator bath and thus the treatment of nuclear tunneling. A comparative discussion of the outcome of these three methods also in relation to experiment [1] is given finally.

[1] Regehly M. et al., J. Phys. Chem. B 2007, 111, 998
[2] Hilczer M. et al., J. Photochem. Photobiol. A 2003, 158, 83
[3] Warshel A. et al., Q. Rev. Biophys. 2001, 34, 4, 563

O 73.3 Thu 15:45 H34

Highly conductive PEDOT:PSS for flexible structured ITO-free solar cells — •Claudia M. Palumbiny[1], Christoph Heller[1], Robert Meier[1], Gonzalo Santoro[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str.1, 85747 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

PEDOT:PSS is widely used as selective intermediate electrode in flexible electronics. The mechanical stability of the electrodes yet play a crucial role and is limited by the instability of the ITO/FTO electrode and the low conductivity of PEDOT:PSS. We investigate a recently developed post treatment method enhancing the conductivity of PEDOT:PSS reaching the order of ITO. For a deeper understanding the nanomorphology is investigated with surface imaging techniques (AFM, SEM) and the inner morphology and crystallinity is addressed with GISAXS and GIWAXS. The morphological changes are consequently related to the electronically changes. Furthermore, we introduce a novel structuring routine for PEDOT:PSS, plasticizer assisted soft embossing [1]. Being able to control the interface between the transparent electrode and the active material, the device efficiency of OPVs under oblique light can be increased. Combining highly conductive PEDOT:PSS with controlled structuring, these results reveal new paths for flexible structured ITO-free solar cells of enhanced efficiency.

[1] R. Meier, C. Birkenstock, C.M. Palumbiny and P. Müller-Buschbaum, Phys. Chem. Chem. Phys., 14, 15088-15098 (2012)

O 73.4 Thu 16:00 H34

Electropolymerized polythiophenes as contact layers in organic solar cells — •Sidhant Bom and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Electropolymerized thiophene offers additional advantages to solution processable thiophenes because the doping concentration can be controlled with electrical parameters. The in-situ electrochemical doping provides a handle for the optimization of organic solar cells, either as a bulk polymer in the active layer or as an electron blocking layer. Here in this study, thiophenes are grown electrochemically with a standard three electrode system on Indium Tin Oxide (ITO) contacts. Characterization by UV-Vis measurements reflects the tunable final oxidation state of the thiophene layer. Thin layers are used in diode configuration using metal contacts like Au, Ag, Al and Cu. Static IV measurement allows the characterization of the contact according to Schottky model. Impedance measurements are used to determine the doping level of the layer. The doping level is found to be systematically depending on the applied negative bias during growth at the working ITO electrode with respect to the counter electrode. Applying a negative bias for a short interval at the end of the growth results in highly doped layers which are suitable for contact layers in solar cells.

O 73.5 Thu 16:15 H34

Efficient solution processed p-type doping for OLEDs — •Christian Töpel, Thorsten Umbach, André Joppich, Jeanette Böckmann, Anne Köhnen, and Klaus Meerholz — University of Cologne, Chemistry Department

Organic light emitting diodes (OLEDs) have drawn much attention in science and industry. Application such as new generation lighting and display devices contribute strongly. However, drawbacks are inefficient charge carrier injection into and low conductivity of the organic materials. A promising solution for this problem is molecular doping which is commonly used in vacuum processed OLEDs, yielding in highly efficient luminescent devices (pin concept). In this case, the molecular doping leads to partial redoxchemical doping. As vacuum deposition is very cost intensive and does not allow high volume processing, researchers focus more and more on solution processing. Here, we present efficient molecular p-type doping using various crosslinkable small-molecule hole transporting materials combined with a range of molecular dopants. Unipolar devices feature an increase in current density by several orders of magnitude compared to the undoped devices at the same voltage. We will also introduce these layers into all-solution-processed multiple-layer OLEDs. These devices are compared with their vacuum-processed counterparts to show the influence of the deposition method and doping ratio on OLED lifetime and device performance.

O 73.6 Thu 16:30 H34

Degradation induced decrease of the radiative quantum efficiency in organic light-emitting diodes — •Tobias D. Schmidt[1], Daniel S. Setz[2], Michael Flämmich[3], Bert J. Scholz[1], Arndt Jaeger[2], Carola Diez[2], Dirk Michaelis[3], Norbert Danz[3], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]OSRAM Opto Semiconductors GmbH, Leibnizstrasse 4, 93055 Regensburg, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

The efficiency decrease during electrical operation of organic light-emitting diodes is a crucial issue for both applied and fundamental research. In order to investigate degradation processes, we have performed an efficiency analysis for phosphorescent state-of-the-art devices in the pristine state and after an accelerated aging process at high current density resulting in a luminance drop to less than 60 % of the initial value. This loss in efficiency can be explained by a decrease of the radiative quantum efficiency of the light-emitting guest/host system from 70 % to 40 %, while other factors determining the efficiency are not affected.

15 min. break

O 73.7 Thu 17:00 H34

Enhanced light outcoupling from corrugated top-emitting OLEDs — •C. Fuchs[1], T. Schwab[1], A. Zakhidov[1,2], K. Leo[1], M. C. Gather[1], and R. Scholz[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden — [2]Fraunhofer COMEDD, Maria-Reiche-Str. 2, 01109 Dresden

We analyse the emission spectra of phosphorescent top-emitting OLEDs grown on corrugated substrates. The corrugation is produced using photolithography. Thereby photoresist, spin-coated on a glass substrate is illuminated by an incoherent UV source across a contact mask with periodic structures in the sub-μm range. The optical microcavity of the OLED grown on top is defined by a thick metallic bottom contact, organic layers following the p-i-n concept, a thin metallic top contact, and an organic capping layer maximizing the outcoupling efficiency. Depending on the periodicity of the substrate, Bragg scattered wave guide modes may interfere constructively or destructively with the cavity mode inside the air light cone, hence enhancing or decreasing light emission with respect to a planar microcavity. Thus, the emission pattern deviates strongly from a Lambertian shape, but the angle-integrated external quantum efficiency can be enhanced by up to a factor of about 1.2 with respect to a fully optimized planar reference. Besides a quantitative assignment of sharp features in the emission spectra, an analysis of Bragg scattering for different periodicities can be used for designing a particular angular emission pattern, e.g. very strong forward characteristics.

O 73.8 Thu 17:15 H34

Characterization of Gravure Printed Polymer Light-Emitting Electrochemical Cells — •Gerardo Hernandez-Sosa, Ralph Eckstein, Serpil Tekoglu, Florian Mathies, Uli Lemmer, and Norman Mechau — Lichttechnisches Institut, Karlsruher Institut für Technologie , Karlsruhe, Deutschland

In this work we present the fabrication, characterization and ink formulation of gravure printed polymer light-emitting electrochemical cells (LECs). These light emitting devices are fabricated by sandwiching a blend of a semiconducting polymer with a solid polymer electrolyte (SPE) between two electrodes, regardless of their work function. When applying a voltage to the device, the ionic species in the active film will help to form p or n doped layers at the corresponding electrode. Following the injection of carriers, the light emission will come from the semiconductor through the formation and successive recombination of excitons in the intrinsic layer between the p and n doped regions. We correlate the LEC ink formulation to the film quality and device performance. The properties of the formulation are characterized by viscosity and contact angle measurements while the properties of the film are studied by impedance spectroscopy and atomic force microscopy.

O 73.9 Thu 17:30 H34

Strongly Fluorescent Copper Complexes for Application in OLEDs Using the Singlet-Harvesting Effect

— •Rafal Czerwieniec and Hartmut Yersin — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040, Germany.

A series of strongly luminescent Cu(I) complexes is presented. The emissions cover a broad spectral range from the blue to the orange. The ambient temperature quantum yields are as high as 90 % and the decay times lie in the order of several microseconds. From a detailed analysis of the photophysical behavior, the ambient temperature emission is assigned to a thermally activated delayed fluorescence (TADF). This is in contrast to the situation at low temperatures, e.g. below 100 K, at which the emission stems from the lowest triplet state decaying as long-lived phosphorescence (order of several hundred microseconds). The observed photophysical properties are related to small energy separations between the S_1 (singlet) and T_1 (triplet) excited states. The results demonstrate the high potential for application of these materials as OLED emitters by exploiting the recently reported singlet harvesting mechanism.

Literature:
1. R. Czerwieniec, J. Yu, H. Yersin, Inorg. Chem., 2011, 50, 8293-8301.
2. H. Yersin, A. F. Rausch, R. Czerwieniec, T. Hofbeck, T. Fischer, Coord. Chem. Rev., 2011, 255, 2622-2652.

O 73.10 Thu 17:45 H34

Insight into the photophysics of photocatalytically active polymeric carbon nitride: an optical quasi-monomer

— •Christoph Merschjann[1], Tobias Tyborski[1,2], Steven Orthmann[1,3], Florent Yang[1], Klaus Schwarzburg[1], Michael Lublow[1,4], and Thomas Schedel-Niedrig[1] — [1]Helmholtz-Zentrum-Berlin für Materialien und Energie — [2]Max-Born-Institut für nichtlineare Optik und Kurzzeitspektroskopie, Berlin — [3]Technische Universität Berlin — [4]Leibnitz-Institut für Katalyse, Rostock

A comprehensive investigation of the luminescent properties of photocatalytically active carbon nitride polymers, based on tri-*s*-triazine units, has been conducted for the first time. Steady-state temperature- and excitation-power-dependent as well as time-resolved measurements with near-UV excitation ($\lambda = 325\,\mathrm{nm}$ & $405\,\mathrm{nm}$) yield strong photoluminescence, covering the visible spectrum. The spectral, thermal and temporal features of the photoluminescence can be satisfactorily described by the excitation and radiative recombination of molecular excitons, localized at single tri-*s*-triazine units. The discussed model is in accordance with the recently reported absorption features of carbon nitride polymers. Thus, from the point of view of optical spectroscopy, the material effectively behaves as a monomer rather than a classical semiconductor.

O 73.11 Thu 18:00 H34

Polymer semiconductors for electro chemical measurements in biosensing applications

— •Martin Schmid — Helmholtz Zentrum München, Munich, Germany

There is an increasing need in medical diagnosis for reliable fast and simple biosensing devices. Sensors based on organic semiconducting polymers, which are suitable for large-area, low-cost, flexible, and eventually single-use throwaway electronics, provide a unique opportunity in that sense. We report on organic field-effect transistors (OFETs) with regioregular poly(3-hexylthiophene) (P3HT) operable at low-voltages in liquid solutions, suitable for in vitro biosensing applications. Measurements in electrolytes have shown that the performance of the transistors did not deteriorate and they can be directly used as ion-sensitive transducers. Here we show the detection of pH alterations in a wide linear range. With the intention to use the sensors as biosensing devices in biomedical applications, the experiments were performed under physiological conditions and temperature.

O 73.12 Thu 18:15 H34

Magnetoresistive Field-Effect Transistors based on Spiro-TAD/Spiro-PFPy Donor/Acceptor-Blends

— •Thomas Reichert, Carolin Isenberg, Tobat Saragi, and Josef Salbeck — Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, 34132, Kassel, Germany.

One promising opportunity for the realization of next generation magnetooptoelectronic devices is the use of the electron spin as an additional control parameter. In organic semiconductors the spin states of quasiparticles can be adjusted with low magnetic fields, which leads to large (up to 20% at 10mT) magnetoresistive effects at room temperature. We show that the sign of magnetoresistance (MR) in organic field-effect transistors (OFETs) can be tuned from positive to negative by simply applying illumination. In darkness an external magnetic-field increases the resistance (positive MR) while a magnetic-field induced resistance decrease (negative MR) can be achieved under illumination. The key aspect of this promising effect is the application of co-evaporated Spiro-TAD/Spiro-PFPy blends as the charge transport layers in OFETs. Due to the hole (electron) stabilizing properties of Spiro-TAD (Spiro-PFPy) a mixed donor/acceptor blend is formed, which leads to the observed photoinduced MR sign change. This effect can pave the way to future multifunctional spintronic devices.

O 73.13 Thu 18:30 H34

In-wire device: combination of organic semiconductors with electrodes in an individual nanowire

— •Chengliang Wang, Huaping Zhao, Liaoyong Wen, Yan Mi, and Yong Lei — Fachgebiet 3D-Nanostrukturierung, Institut fur Physik & IMN MacroNano* (ZIK), Technische Universitaet Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany

One-dimensional wires constituted with kinds of segments attracted much attention due to the their potential application in nanogaps obtained from on-wire lithography, plasmonic disk arrays, optimized Raman *hot spots* and heterojuction structures1. Here, we will talk about the in-wire device, which combined the organic semiconductor and the electrodes in an individual nanowire, based on anodic alumina oxide (AAO) template2-3. This kind of nanodevice could be applied in organic diodes, transistors or memories, which attracted extensive attention due to the flexibility, the ease to be functionalized, the colorful and the low cost4.

Reference:

[1] S. J. Hurst, E. K. Payne, L. Qin, C. A. Mirkin, Angew. Chem. Int. Ed. 2006, 45, 2672.

[2] Y. Lei, S. Yang, M. Wu, G. Wilde, Chem. Soc. Rev. 2011, 40, 1247.

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[4] C. Wang, H. Dong, W. Hu, Y. Liu, D. Zhu, Chem. Rev. 2012, 112, 2208.

O 74: Focussed Session: Frontiers of Electronic Structure Theory VII (jointly with HL and TT)

Time: Thursday 16:00–19:00 Location: H36

O 74.1 Thu 16:00 H36

Determination of the one-body Green's function: freedom and constraints

— Giovanna Lani[1,4], •Pina Romaniello[2,4], and Lucia Reining[3,4] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Laboratoire de Physique Théorique-IRSAMC, CNRS, Université Paul Sabatier, Toulouse, France — [3]Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, Palaiseau, France — [4]European Theoretical Spectroscopy Facility (ETSF)

The one-particle Green's function G plays a key role in many-body physics due to the wealth of physical information that it contains. In this work we go beyond the standard methods to calculate G, which are plagued by various shortcomings, and we use an approximate set of functional differential equations relating the one-particle Green's function to its functional derivative with respect to an external perturbing potential [1]. We show that this set of equations has, in principle, multiple solutions, but that only one is well behaved - this is the physical solution. We give the formally exact family of solutions, which depends on an auxiliary quantity q, for which we find stringent exact constraints. Our findings suggest that once q is known, the physical solution is uniquely fixed by the vanishing Coulomb interaction limit [2-3].

[1] L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics (W.A. Benjamin Inc., New York, 1964)
[2] G. Lani, P. Romaniello, and L. Reining, New Journal of Physics, 14, 013056 (2012)
[3] G. Lani, P. Romaniello, and L. Reining, in preparation

O 74.2 Thu 16:15 H36

Restoring piecewise linearity in density-functional theory — •Ismaila Dabo[1], Andrea Ferretti[2], Matteo Cococcioni[3], and Nicola Marzari[4] — [1]Ecole des Ponts ParisTech, Marne-la-Vallee, France — [2]CNR-Istituto Nanoscienze, Modena, Italy — [3]University of Minnesota, Minneapolis, USA — [4]EPFL, Lausanne, USA

Electronic-structure calculations based upon density-functional theory (DFT) have been fruitful in diverse areas of condensed matter physics. Despite their exceptional success, it can hardly be denied that a range of fundamental electronic properties fall beyond the scope of current DFT approximations. Many of the failures of DFT calculations take root in the lack of piecewise linearity of approximate functionals, which reverberates negatively on the electronic-structure description of systems involving fractionally occupied and spatially delocalized electronic states, including but not restricted to dissociated molecules, adsorbed species, charge-transfer complexes, and semiconducting compounds. In this talk, I will present a novel class of first-principles methods that restores the piecewise linearity of the total energy by imposing Koopmans' theorem to DFT approximations. The Koopmans-compliant approach is apt at describing full orbital spectra within a few tenths of an electron-volt relative to experimental direct and inverse photoemission data. This level of accuracy is comparable to the predictive performance of accurate many-body perturbation theory methods at a fraction of their computational cost, and with the additional benefit of providing accurate total energies for systems with fractional occupations.

O 74.3 Thu 16:30 H36

Self-interaction-corrected and Koopmans-compliant functionals: from molecules to solids — •Giovanni Borghi[1], Linh Nguyen[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, EPFL, Lausanne — [2]CNRNANO, University of Modena and Reggio Emilia — [3]Ecole des Ponts ParisTech, Université Paris-Est

We present an overview of the performance of self-interaction corrected, orbital-density dependent functionals as applied to the calculation of the electronic structure of atoms, molecules and solids.

In particular, we show how orbital-dependent corrections of Koopmans' compliant functionals are able to restore not only the correct ionization energies, but also the eigenvalues of low-lying single-particle states with an accuracy comparable or better to that of many-body perturbation theory, while retaining a variational principle which grants the possibility to optimize geometries and bond lengths.

The outcome of these orbital-density dependent calculation remain, even in the thermodynamic limit, Wannier-like orbitals, that localize thanks to a condition related to the Edmiston-Ruedenberg criterion. These localized functions can be used as Wannier interpolators of band structures, allowing to discuss the performance of the functionals in the solid-state limit.

O 74.4 Thu 16:45 H36

Lattice density functional theory at finite temperature with strongly density-dependent exchange-correlation potentials — •Stefan Kurth[1], Gao Xianlong[2], A-Hai Chen[2], and Ilya Tokatly[1] — [1]Univ. of the Basque Country UPV/EHU, San Sebastian, Spain and IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [2]Zhejiang University, Jinhua, China

The derivative discontinuity of the exchange-correlation (xc) energy of density functional theory (DFT) at integer particle number is absent in many popular local and semilocal approximations. In lattice DFT, approximations exist which exhibit a discontinuity in the xc potential at half filling but due to convergence problems of the Kohn-Sham (KS) self-consistency cycle, the use of these functionals is mostly restricted to situations where the local density is away from half filling. Here a numerical scheme for the self-consistent solution of the lattice KS Hamiltonian with a local xc potential with rapid (or quasi-discontinuous) density dependence is suggested. The problem is formulated in terms of finite-temperature DFT where the discontinuity in the xc potential emerges naturally in the limit of zero temperature. A simple parametrization is suggested for the xc potential of the uniform 1D Hubbard model at finite temperature obtained from the thermodynamic Bethe ansatz. The feasibility of the numerical scheme is demonstrated by application to a model of fermionic atoms in a harmonic trap. The corresponding density profile exhibits a plateau of integer occupation at low temperatures which melts away for higher temperatures.

O 74.5 Thu 17:00 H36

Kohn-Sham equations beyond the single-determinant approximation — Nektarios N. Lathiotakis[1], •Nicole Helbig[2,3], Nikitas I. Gidopoulos[4], and Angel Rubio[3,5] — [1]Theoretical and Physical Chemistry Institute, NHRF, Athens, Greece — [2]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany — [3]Nano-Bio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC and DIPC, San Sebastián, Spain — [4]ISIS, STFC, Rutherford Appleton Laboratory, HSIC, Didcot, United Kingdom — [5]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We describe a new method for the optimization of the total energy in reduced density matrix functional theory (RDMFT) which reduces the computational costs to the costs of a density functional calculation within the optimized effective potential method. Within this method the natural orbitals are restricted to be solutions of a single-particle Schrödinger equation with a local effective potential which in addition to reducing the computational costs also provides an energy eigenvalue spectrum connected to the natural orbitals. This energy spectrum is shown to reproduce the ionization potentials of different atoms and molecules very well. In addition, the dissociation limit is well described without the need to break any spin symmetry, i.e. this attractive feature of RDMFT is preserved.

O 74.6 Thu 17:15 H36

Initial stages of time-evolution of excitations in Fermi liquids and finite systems — •Yaroslav Pavlyukh[1], Jamal Berakdar[1], and Angel Rubio[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. de Física de Materiales, Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC and DIPC, Av. Tolosa 72, E-20018 San Sebastián, Spain

A particle-hole excitation in a many-body system is not an eigenstate and, thus, evolves in time. The evolution at short times after an excitation with the energy ϵ was created is the quadratic decay with the rate constant $\sigma^2(\epsilon)$. Later, after some set-in time $\tau(\epsilon)$, the exponential decay develops. It is governed by another rate constant $\gamma(\epsilon)$.

We study the electron-boson model for the homogenous electron gas and use the first order (in boson propagator) cumulant expansion of the electron Green's function. In addition to a quadratic decay in time upon triggering the excitation, we identify non-analytic terms in the time expansion similar to those found in the Fermi edge singularity phenomenon.

Finite systems (J. Chem. Phys., **135**, 201103 (2011)) give an opportunity to test the conjectured behavior numerically as an exact solution of a many-body problem is feasible. We propose a simple model for the electron spectral function that links together all three aforementioned parameters and give a prescription how the energy uncertainty $\sigma^2(\epsilon)$ can be computed within the many-body perturbation theory.

O 74.7 Thu 17:30 H36

Real-structure effects from *ab-initio* calculations — •Andre Schleife — Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, Livermore, CA, USA

By harnessing the power of supercomputers, *computational materials science* is becoming a field that enables insight into fundamental materials physics. It is inevitable to further push *ab-initio* approaches, allowing them to account for effects that are important at the forefront of experimental research.

I will present the solution of the Bethe-Salpeter equation as a recent theoretical-spectroscopy technique and how it is extended and used to understand real-structure effects in oxide and nitride semiconductors. This talk will illustrate the success of our modification of this framework to describe the interplay of free electrons and excitonic effects in *n*-doped ZnO. Combining a cluster expansion scheme and electronic-structure calculations allows to explore the potential for band-gap tailoring in oxide and nitride alloys. These material systems are a driving force of current semiconductor technology, e.g. for solar cells and solid-state lighting; understanding fundamental effects will help to overcome performance limits.

In addition, computational materials science can *replace* dangerous experiments, e.g. in the context of radiation damage: I will present large-scale simulations of non-adiabatic electron-ion dynamics based on real-time time-dependent density functional theory that explain electronic stopping as an important mechanism responsible for radiation damage when fast H or He ions penetrate aluminum.

O 74.8 Thu 17:45 H36

Specwer: an efficient first-principle program for electronic structures and spectroscopic simulations of nanomaterials — •Bin Gao — Center for Theoretical and Computational Chemistry, Department of Chemistry, University of Tromso, N-9037 Tromso, Norway

Although nanomaterials have been routinely synthesized and analyzed in various laboratories around the world, they still present great challenges for theoretical studies using the ab initio and/or first-principle methods due to the simple fact that they are too large to handle for the conventional theoretical approaches. Various linear-scaling methods have been proposed in recent decades to circumvent this difficulty. In this talk, I will present our recently developed program Specwer and its applications for electronic structures and spectroscopic simulations of different nanomaterials. For large-scale molecules, Specwer program employs the reduced single-electron density matrix and divide-and-conquer method. I will show its applications in the ground and excited states of nanomaterials at various density functional theory levels, in which the information of excited states is obtained via solving the so-called Liouville-von Neumann equation. I will also highlight the importance of including the spin-orbit coupling in some cases, for instance, the L-edge X-ray absorption spectroscopy, and the electron transport in double-stranded DNA molecules.

O 74.9 Thu 18:00 H36

Generalized incomplete-basis-set correction applied to EXX-OEP — •Markus Betzinger, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We recently derived [1] an incomplete-basis-set correction (IBC) for all-electron response functions within the full-potential linearized augmented plane-wave (FLAPW) method as realized in the `FLEUR` code [2]. The IBC utilizes the potential dependence of the LAPW basis functions whose response is calculated explicitly by solving radial Sternheimer equations in the spheres. While in the original formulation of the IBC [1] only spherical perturbations of the potential have been taken into account, we show here an extension to non-spherical perturbations, replacing the single radial Sternheimer equation for each angular momentum ℓ by a set of equations coupling different angular momenta. Likewise, the response of the core electrons is computed. We demonstrate that this generalized IBC improves further the convergence in terms of basis-set size and number of unoccupied states. We apply the generalized IBC to the exact-exchange (EXX) optimized-effective-potential (OEP) approach. While for simple semiconductors and insulators the original IBC already leads to a physical and stable local EXX potential, we show that for more complex materials like NiO, whose band gap is formed by *d* states, the generalization of the IBC is crucial to obtain a well-converged local optimized potential.

[1] M. Betzinger *et al.*, Phys. Rev. B **85**, 245124 (2012)

[2] http://www.flapw.de

O 74.10 Thu 18:15 H36

One particle spectral function and analytic continuation for many-body implementation in the exact muffin-tin orbitals method — •Andreas Östlin[1], Liviu Chioncel[2,3], and Levente Vitos[1,4,5] — [1]Department of Materials Science and Engineering, Applied Materials Physics, KTH Royal Institute of Technology, Stockholm SE-100 44, Sweden — [2]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [4]Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-751210, Uppsala, Sweden — [5]Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest H-1525, P.O. Box 49, Hungary

We investigate one of the most common analytic continuation techniques in condensed matter physics, namely the Padé approximant. Aspects concerning its implementation in the exact muffin-tin orbitals (EMTO) method are scrutinized with special regard towards making it stable and free of artificial defects. We discuss the difference between the **k**-integrated and **k**-resolved analytical continuations, as well as describing the use of random numbers and pole residues to analyze the approximant. It is found that the analytic properties of the approximant can be controlled by appropriate modifications. At the end, we propose a route to perform analytical continuation for the EMTO + dynamical mean field theory (DMFT) method.

O 74.11 Thu 18:30 H36

Core-electron forces within the FLAPW method — •Daniel Aaron Klüppelberg, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The full-potential linearized augmented-plane-wave method (FLAPW) is an all-electron electronic-structure method based on density functional theory (DFT). Characteristic to the method is that space is divided into spheres around the atoms, so called 'muffin-tins', and an interstitial region in between. Local orbitals can be used to describe semicore states within the valence-state formalism. It is established as an accurate tool for describing many properties of complex materials.

We address the occurrence of contributions to the forces due to core electrons described by wave functions having tails exceeding the muffin-tin boundary. Accurate forces are needed not only for relaxing the atomic structure to its ground state, but also in order to calculate precise phonon spectra via the finite-displacement method. We present a core-tail correction to the Pulay force term found by Yu *et al.* [1], implemented into the `FLEUR` code [2], which deals with the core electrons. This addition extends the known formula over the whole unit cell and therefore includes the complete force contribution coming from core states that extend beyond their muffin-tin. In this talk, we will present examples on the performance of this addition in comparison to the inclusion of local orbitals and the adjustment of the muffin-tin radii.

[1] R. Yu, D. Singh, and H. Krakauer, Phys. Rev. B **43**, 6411 (1991)

[2] www.flapw.de

O 74.12 Thu 18:45 H36

The linearized augmented lattice-adapted plane wave basis — •Gregor Michalicek and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The full-potential linearized augmented plane wave method (FLAPW) is an all-electron electronic structure method that provides density functional results for complex solids with very high precision, irrespective of the chemical element of the solid. For this purpose the Kohn-Sham wavefunctions are expanded into LAPW basis functions. These are plane waves in an interstitial region (IR) that are augmented by atom-centered functions in non-overlapping spheres around each atom. The LAPW basis features many desirable properties that are a key component to the high precision of the FLAPW method.

In this talk we show that the capability of the FLAPW method can be kept with a modification of the basis-set that is numerically more efficient. We argue that the required plane-wave cut-off of the interstitial part of the LAPW basis results mostly from mathematical conditions and the efficiency of the LAPW description can be increased by incorporating more physics into the construction of this part of the basis. We propose a linearized augmented lattice-adapted plane wave basis ($(\mathrm{LA})^2\mathrm{PW}$) that replaces the plane waves in the IR by smart linear combinations of plane waves, show how to realize an efficient implementation of such a basis, and provide a construction principle for the linear combination of plane waves. The so constructed basis is evaluated in terms of precision and calculation runtime performance.

O 75: Organic/bio Molecules on Metal Surfaces VI

Time: Thursday 16:00–19:15 Location: H38

O 75.1 Thu 16:00 H38

Bonding and chemical transformations of free-base porphyrin species on Ag(111) — •Alissa Wiengarten, Knud Seufert, Willi Auwärter, David Écija, Sushobhan Joshi, and Johannes V. Barth — Physik Department E20, Technische Universität München, D-85748 Garching, Germany

Porphyrins play a key role in many biological processes and are promising building blocks for technical applications. Depending on their substitution and the variation of the metal-center incorporated into the macrocycle, the functionality of these molecules can be tuned. A starting point for a systematic investigation of this class of molecules is the fundamental building block for all porphyrin derivatives, the free-base porphine, forming the macrocycle. In this work we study temperature-induced covalent coupling of free-base porphines on the Ag(111) surface via low temperature scanning tunneling microscopy (LT-STM) in ultra high vacuum (UHV). We find that porphines can dehydrogenate and form direct C-C bonds on a hot surface. With increasing sample temperature the number of covalently bound oligomers increases. A further step focuses on the investigation of tetraphenyl-porphyrins on Ag(111), where the molecule shows a so called saddle-shape deformation. Similar to the porphine case annealing induces dehydrogenation reactions resulting in the formation of different porphyrin-derivatives lying flat on the surface.

O 75.2 Thu 16:15 H38

Tuning the Kondo screening of an Fe-Porphyrin molecule by *on-surface* ligand modification — •Benjamin W. Heinrich[1], Gelavizh Ahmadi[1], Valentin Müller[1], José I. Pascual[1,2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]CIC nanoGUNE, 20018 Donostia-San Sebastián, Spain

The structure of the organic ligand in metal-organic complexes governs the adsorption on a metal surface, and thereby, the magnetic interaction between the central ion and the conduction electrons. We use Scanning Tunneling Microscopy and Spectroscopy (STM/STS) at 4.5 K to show how the modification of the ligand structure alters the Kondo screening of an Fe-Porphyrin on Au(111). Annealing Fe(II)-Octaethylporphyrin (FeOEP) on Au(111) to temperatures of about 470 K, we step-wise induce an electrocyclic ring closure of the ethyl groups to finally produce Fe-Tetrabenzoporphyrin (FeTBP). In STS, complex features at low energies around the Fermi level result from Kondo screening of the iron ion's spin. Changes in width and shape show the tuned interaction of the local spin with the conduction electrons depending on the actual chemical structure of the ligand. These results highlight the importance of chemical engineering for controlling the magnetism of single molecules on surfaces.

O 75.3 Thu 16:30 H38

Temperature-Dependent Chemical and Structural Transformations from 2H-Tetraphenylporphyrin to Copper(II)-Tetraphenylporphyrin on Cu(111) — •Stefanie Ditze, Michael Stark, Jie Xiao, Michael Röckert, Martin Drost, Florian Buchner, Ole Lytken, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

Temperature-driven chemical and structural changes of 2H-Tetraphenylporphyrin (2HTPP) adsorbed on Cu(111) have been investigated by a combination of scanning tunneling microscopy (STM) and X-ray photoemission spectroscopy (XPS) under UHV conditions. The first chemical change is a redox reaction of the porphyrin center with Cu atoms from the substrate, resulting in the formation of Copper(II)-Tetraphenylporphyrin (CuTPP). For a coverage of about 0.17 molecules/nm^2, this reaction was found to start around 400 K and can easily be monitored by STM, due the very different adsorption behavior of 2HTPP and CuTPP on Cu(111). The energetic parameters of this self-metalation reaction were determined by isothermal STM experiments.[1] Subsequent annealing to 450 and 500 K leads to two intramolecular structural changes, which are attributed to successive dehydrogenation reactions of CuTPP.[2]

This work has been funded by the DFG through SFB 583.

[1] S. Ditze et al.Angew. Chem. Int. Ed. 2012, 51, 10898-10901 [2] Xiao et al. J. Phys. Chem. C 2012, 116, 12275-12282

O 75.4 Thu 16:45 H38

Coverage-dependent metalation of tetraphenylporphyrin with Cu(111) — •Michael Röckert, Jie Xiao, Stefanie Ditze, Michael Stark, Mathias Grabau, Hubertus Marbach, Hans-Peter Steinrück, and Ole Lytken — LS für PC II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen

The coverage-dependent metalation of tetraphenylporphyrin (2HTPP) with Cu atoms from a Cu(111) substrate has been investigated by X-ray photoemission spectroscopy (XPS) and scanning tunneling microscopy (STM) from submonolayer to multilayer coverages. At coverages below 0.17 molecules/nm^2 the rate of metalation is modest and follows a first order behaviour. However, as the coverage is increased beyond 0.35 molecules/nm^2 a strong increase in the rate of metalation is observed, and the rate no longer follows a simple first order behaviour. This behaviour is accompanied by the appearance of a checkerboard structure at coverages above 0.35 molecules/nm^2 as found by STM. Temperature-dependent rates of metalation have been measured for both high ($>$0.35 molecules/nm^2) and low ($<$0.35 molecules/nm^2) coverage, and, based on Arrhenius analyses, prefactors and activation energies for the two reaction channels have been extracted. It was found that the metalation reaction for the high-coverage checkerboard structure had a significantly lower activation energy compared with coverages below 0.17 molecules/nm^2. The reason for the increased reactivity could be easier access of copper adatoms to the slightly elevated porphyrin molecules in the checkerboard structure.

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O 75.5 Thu 17:00 H38

Ab initio study of CoTPP on coinage metal surfaces — •Torsten Houwaart and Marie-Laure Bocquet — Laboratoire de Chimie, 46 allée d'Italie, 69364 Lyon cedex 07

Metal-Tetra-Phenyl-Porphyirins (MeTPP) are large π-conjugated molecules which are prevalent in nature. These molecules have applications in many fields of physics and chemistry. We analyze MeTPPs on metallic substrates for its possible application as a gas sensing system or in optoelectronics.

From Scanning-Tunneling-Microscopy experiments it is well known that MeTPPs undergo a deformation on a metallic substrate. We analyze the geometry of the molecule after adsorption as the deformation of porphyrins from a planar shape is believed to have an influence on the reactivity. In this ab-initio study with the density functional code VASP we analyzed the binding site of Cobalt-TPP on Cu(111) with the local density approximation (LDA) and the generalized gradient approximation (GGA) of Perdew, Burke and Ernzerhof (PBE) with and without semi-empirical dispersion (D2) correction by Grimme. From a theoreticians point of view it is important to understand the effect of using different exchange-correlation functionals for the calculation of these systems and the resulting geometries and electronic structure. By looking at changes to the electronic structure of the system the bonding mechanisms on the different binding sites were analyzed.

O 75.6 Thu 17:15 H38

Investigation of the influence of hydrogen bonding on the self-assembled molecular adsorbate structure and manipulation of the electronic structure of tetra(p-hydroxyphenyl)porphyrin — •Lars Smykalla[1], Michael Hietschold[1], Carola Mende[2], and Heinrich Lang[2] — [1]Chemnitz University of Technology, Institute of Physics, D-09107 Chemnitz, Germany — [2]Chemnitz University of Technology, Institute of Chemistry, D-09107 Chemnitz, Germany

Combining scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), photoemission spectroscopy (PES) and density functional theory (DFT), we present a thorough study of the adsorption of tetra(p-hydroxyphenyl)porphyrin (H_2THyPP) on crystalline metal substrates. The observed molecular arrangements on Au(111) and the more anisotropic Ag(110) are explained in terms of epitaxy and intermolecular weak hydrogen bonding. Furthermore, the influence of the substrates on the electronic structure of the adsorbed molecules is discussed. The electronic states of the molecule are studied with high spatial resolution using voltage-dependent STM and STS in ultra-high vacuum, whereby two different kinds of molecular appearances at constant voltage in a monolayer are observed. Further, we are able to switch the molecular contrast of single molecules under the STM tip by voltage pulses. To understand the nature of this change in electronic structure of the molecule we applied density functional theory calculations, which indicate that we find on the surfaces the free-base H_2THyPP as well as its deprotonated form (without the two hydrogen atoms in the center of the molecule).

O 75.7 Thu 17:30 H38

Assembly, electronic structure and metal-ligand interaction of di-carbonitrile quaterphenyls on an electronically corrugated boron nitride monolayer. — •Tobias Hoh[1], Sushobhan Joshi[1], Willi Auwärter[1], Carlos-Andres Palma[1], Florian Klappenberger[1], David Écija[1], Alissa Wiengarten[1], Hermann Sachdev[2], and Johannes V. Barth[1] — [1]Physik Department, E20, TU München, Germany — [2]Max-Planck-Institut für Polymerforschung, Germany

Metal-directed assembly at interfaces is important for the engineering of nanostructures. For molecules on metal surfaces, the presence of substrate electrons can lead to strong perturbations of the electronic structure and unique coordination motifs. Here, we present a low temperature scanning tunneling microscopy(STM) study of di-carbontitrile quaterphenyl molecules on an insulating boron nitride(BN) monolayer grown on Cu(111)[1]. The molecules form a dense packed chevron assembly in contrast to open porous pattern observed on Ag(111)[2]. STM images show a nonplanar conformation corroborated by a molecular dynamics simulation. Tunneling spectroscopy evidences decoupling of the molecules from the metal. Moreover, the inhomogenous BN template induces a spatial modulation of the energy of unoccupied molecular orbitals. A subsequent deposition of cobalt atoms generates a four-fold coordination motif.

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

[2] Schlickum, V. et al., J. AM. CHEM. SOC. 2008, 130, 11778-11782

O 75.8 Thu 17:45 H38

2D lanthanide networks — •Jose I. Urgel[1], David Ecija[1], Anthoula C. Papageorgiou[1], Saranyan Vijayaraghavan[1], Sushobhan Joshi[1], Willi Auwärter[1], Svetlana Klyatskaya[2], Mario Ruben[2], Sybille Fischer[1], Joachim Reichert[1], and Johannes V. Barth[1] — [1]Physik Department E20, Technische Universität München, D-85748 Garching, Germany — [2]Karlsruhe Institut für Technologie D-76344 Eggenstein-Leopoldshafen, Germany

Surface-confined metal organic architectures have been recently studied for alkali and transition metals in 2D. However, the field of lanthanide based networks on surfaces remains largely unexplored. Here we present, using scanning tunneling microscopy (STM), a distinct coordination of dicarbonitrile-oligophenyl linkers (p-NC-(Ph)n-CN-p (n=3,4)) to cerium centers on Ag (111), exhibiting a flexible five-fold nodal motif. By carefully tuning the concentration and the stoichiometric ratio of the rare-earth metal centers and molecular linkers, we realized a 2D hierarchic metal-organic assembly based on dodecameric units. For an increase in the cerium supply, a fully reticulated 2D metal-organic network evolves, whereby linkers are connected on both sides to Ce centers, following a design pattern identified as a molecular Archimedean snub square tessellation of the surface. Our study introduces the first implementation of the f-block elements in 2D metallosupramolecular assembly.

O 75.9 Thu 18:00 H38

Molecular structure elucidation by atomic force microscopy — •Bruno Schuler, Leo Gross, Fabian Mohn, and Gerhard Meyer — IBM Research - Zurich, 8803 Rueschlikon, Switzerland

Atomic force microscopy (AFM) offers a completely new and direct approach to investigate the chemical structure of individual molecules [1,2] beside commonly used characterization methods including mass spectrometry, spectroscopic techniques or X-ray crystallography. The capabilities and challenges of AFM-based molecular structure identification were demonstrated on a natural product with previously unknown structure. By combining standard experimental and computational techniques together with AFM the structure was solved and revealed a new structural molecule class [3]. The molecule was studied in UHV at low temperatures on a Cu(111) substrate partially covered with a thin film of NaCl. We used noncontact AFM in the dynamic mode [4] and a qPlus force sensor design [5], where the tip apex was functionalized with a CO molecule [6].

References:

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

[2] L. Gross et al., Nature Chem. 2, 821 (2010)

[3] K.O. Hanssen et al., Angew. Chem. Int. Ed. 51 (2012)

[4] T.J. Albrecht et al., Appl. Phys. 69, 668 (1991)

[5] F.J. Giessibl, Appl. Phys. Lett. 73, 3956 (1998)

[6] L. Bartels et al., Phys. Rev. Lett. 80, 2004 (1998)

O 75.10 Thu 18:15 H38

Force and conductance of contacts to a C_{60} molecule — •Nadine Hauptmann[1], Fabian Mohn[2], Leo Gross[2], Gerhard Meyer[2], Thomas Frederiksen[3], and Richard Berndt[1] — [1]Institut für Exp. und Angew. Physik der Universität Kiel (IEAP), D-24098 Kiel, Germany — [2]IBM Research – Zurich, 8803 Rüschlikon, Switzerland — [3]Donostia International Physics Center (DIPC), E-20018 Donostia-San Sebastián, Spain

When a single molecule is contacted to measure its conductance new bonds are formed and significant forces may arise. These forces affect the atomic-scale junction geometry, which is crucial for its transport properties. We present simultaneously measured low-temperature force and conductance data from controlled Cu-C_{60} and C_{60}-C_{60} contacts with submolecular resolution. The contact conductances reported in prior works are shown to correspond to the junction being under maximal tensile stress. In order to estimate relaxations we fit the calculated conductance for a rigid system to the experimental data considering an effective spring constant for the molecular junction. The results indicate that most of the deformation in a Cu-C_{60} contact may be ascribed to relaxations of the Cu tip.

O 75.11 Thu 18:30 H38

Simulation of C60 non-equilibrium surface growth — •Nicola Kleppmann[1], Sebastian Bommel[2,3], Stefan Kowarik[3], and Sabine H. L. Klapp[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Kinetic Monte Carlo simulation methods allow the simulation of non-equilibrium epitaxial surface growth over experimentally realized time spans of minutes and growth of multiple layers of particles [1]. Through variation of simulated temperature and adsorption rate the structures formed can be manipulated and predictions for experimental methods such as molecular beam epitaxy can be made. We apply the method to simulate multilayer growth of C60. The material parameters are obtained through comparison with Grazing-Incidence X-ray Scattering measurements [2]. The simulations allow for a time-resolved analysis of the real and reciprocal surface, geometric and statistical analysis as well as an understanding of microscopic processes obtained from particle trajectories. Characteristic time-dependent features such as the average island distance and layer filling fraction are consistent with the experimental data for long time spans and several temperatures.

[1] A. Chatterjee and D. G. Vlachos, J. Comp.-Aided Mater. Des. 14, 253-308 (2007)

[2] S. Kowarik, A. Gerlach, S. Sellner, F. Schreiber, L. Cavalcanti and O. Konovalov, Phys. Rev. Lett. 96, 125504 (2006)

O 75.12 Thu 18:45 H38

Adsorption site determination of a molecular monolayer via inelastic tunneling — •Daniel Wegner[1,2], Ryan Yamachika[2], Xiaowei Zhang[2], Yayu Wang[2], Michael F. Crommie[2], and Nicolás Lorente[3] — [1]Physikalisches Institut and CeNTech, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]University of California at Berkeley and Lawrence Berkeley National Laboratory, Berkeley, California 94720-7300, USA — [3]Centre d'Investigació en Nanociència i Nanotecnologia, CIN2 (CSIC-ICN), 08193 Bellaterra, Spain

We have combined scanning tunneling microscopy (STM) with inelastic electron tunneling spectroscopy (IETS) and density functional theory (DFT) to study a tetracyanoethylene (TCNE) monolayer on Ag(100). Images show that the molecules arrange in locally ordered patterns with three non-equivalent, but undeterminable, adsorption sites. While scanning tunneling spectroscopy (STS) only shows subtle variations of the local electronic structure at the three different positions, we find that vibrational modes are very sensitive to the local atomic environment. IETS detects sizeable mode frequency shifts of the molecules located at the three topographically detected sites, which permits us to determine the molecular adsorption sites through identification with DFT calculations. This proof-of-principle study shows that IETS combined with DFT can be used to discriminate between non-equivalent molecular adsorption environments in a dense complex molecular monolayer that lacks long-range order and thus would be challenging to study using diffraction-based techniques.

O 75.13 Thu 19:00 H38

Chemisorbed Monolayers of Corannulene Penta-Thioethers on Gold — •Polina Angelova[1], Ephrath Solel[2], Galit Parvari[2], Andrey Turchanin[1], Mark Botoshansky[2], Ehud Keinan[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems and Surfaces, University of Bielefeld, Germany, — [2]Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Haifa 32000, Israel

Corannulene pentathioethers form highly stable monolayers on gold surfaces, as indicated by X-ray photoelectron spectroscopy (XPS). Formation of these homogeneous monolayers involves multivalent coordination of the five sulfur atoms to gold with the peripheral alkyl or aryl substituents pointing away from the surface. No dissociation of C-S bonds upon binding could be observed at room temperature. The XPS experiments reveal strong chemical bonding between the thioether groups and gold, comparable to the bonding between thiolates and gold surfaces. Temperature-dependent XPS study shows that the thermal stability of the monolayers is higher than the typical stability of self-assembled monolayers (SAMs)of thiolates on gold.

O 76: Focussed Session: Solid-liquid Interfaces II

Time: Thursday 16:00–19:00 Location: H31

Topical Talk O 76.1 Thu 16:00 H31

The origin of the high oxygen reduction activity on PtX (X= Sc, Y, La, Sm, Gd and ..) alloys and their activation mechanism. — •Ib Chorkendorff — Technical University of Denmark, Kgs. Lyngby, Denmark

There is a strong demand for improving the anode material of the Proton Exchange Membrane Fuel Cell, either by increasing the activity and thereby being able to reduce the loading or by replacing Pt entirely. Recently we have found a new class of alloys, which are very active towards the Oxygen Reduction Reaction (ORR). The first catalyst were predicted in a DFT screening study which pointed for activity and stability towards Pt3Sc and Pt3Y and the latter proved particular active by a factor 7-8 times as active as polycrystalline Pt. We have since expanded the number of catalyst to also include Zr, Hf, and La, but the most active and stable catalysts seems to be Pt5Ga. By comparison to our recent studies of PtCu catalyst it is possible to identify the surface composition more accurately. The Pt and Y, La, and Gd catalysts are among the most active and stable forming a rather thick skin consisting of several monolayers of Pt. This skin is found to be under compression (although the bulk alloy is expanded compared to pure Pt) leading to the necessary lower binding energy of oxygen explaining the enhanced ORR activity. The skin formation has been investigated by a broad range of surface science methods and the progress concerning the combination of ORR activity and structural investigation of polycrystalline, single crystal, and mass selected nanoparticles will be discussed.

O 76.2 Thu 16:30 H31

Broadband SFG Spectroscopy of Specific Anion Adsorption at Pt(111)-Electrolyte Interfaces — •Björn Braunschweig — University of Erlangen-Nuremberg, Institute of Particle Technology (LFG)

Vibrational broadband sum-frequency generation (SFG) synchronized with cyclic voltammetry (CV) was applied to study the electrochemical adsorption of (bi)sulfate and formate anions on ordered Pt(111) electrodes. SFG spectra of Pt(111) immersed in 0.1 M H_2SO_4 reveal an intense vibrational band at $1270\,\mathrm{cm}^{-1}$ for potentials >0.21 V vs. Ag/AgCl. A close comparison of SFG spectra with in-situ STM images and the CV reveals that this potential corresponds to a surface transformation from a disordered (bi)sulfate adlayer to an ordered layer with large domains of closed-packed $(\sqrt{3} \times \sqrt{7})$R19.1° superstructures [1,2]. Changing the electrode potential results in significant Stark tuning of the (bi)sulfate band and to a second abrupt change in SFG amplitude, bandwidth and Stark tuning rate at 0.5 V that is indicative for a second surface transformation.

In addition to experiments in blank H_2SO_4 dilutions, the adsorption of formate during the electrochemical oxidation of 0.5 M formic acid on Pt(111) has been studied with SFG. For potentials <0.3 V, CO is the dominant surface-adsorbed species, while potentials >0.3 V lead to co-adsorption of formate. Oxidative removal of CO at potentials >0.5 V leads to predominant adsorption of formate.

[1] Braunschweig, Dlott, Wieckowski et al.; JACS, 132, 14036 (2010)
[2] Braunschweig and Daum; Langmuir 25, 11112 (2009)

O 76.3 Thu 16:45 H31

Pt based PEMFC catalysts from colloidal particle suspensions - a toolbox for model studies — •Jozsef Speder[1], Lena Altmann[2], Marcus Bäumer[2], Jacob Kirkensgaard[1], Kell Mortensen[1], and Matthias Arenz[1] — [1]University of Copenhagen — [2]University of Bremen

Polymer membrane fuel cells (PEMFCs) represent a key technology for clean, efficient and sustainable energy conversion. One of the main problems in PEMFCs, however, is the sluggish oxygen reduction reaction (ORR). The objective of our work is to prepare and study model catalysts that can help to understand and thereby improve the existing commercially available electrocatalysts. A typical PEMFC catalyst consists of high surface area carbon supported Pt or Pt-alloy nanoparticles. Previous studies report sometimes with contradicting conclusions on the influence of the support, particle size and composition on the ORR activity. In general however, these studies do not selectively change only one of the variables, for example the Pt loading, while leaving the others constant, e.g. the particle size. In our work we introduce a reliable, artefact-free method for studying these effects by synthesising carbon supported, Pt based catalysts from colloidal dispersions of well defined Pt NPs synthesized by an ethylene glycol method. We demonstrate that this preparation method enables a controlled synthesis of model catalysts where individual parameters such as support material and Pt loading can be tuned without changing other parameters. Thus for example the role of support material, Pt loading etc. can be investigated separated from each other.

15 min. break

Topical Talk O 76.4 Thu 17:15 H31

Coupling electrochemistry to an ICP-MS - online-investigation of electrode material dissolution — •Karl Mayrhofer, Serhiy Cherevko, Angel Topalov, Anna Schuppert, Josef Meier, Aleksandar Zeradjanin, and Ioannis Katsounaros — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Continuous electrochemical flow reactors for efficient conversion of electrical energy into chemicals and vice versa, i.e. fuel cells and electrolyzers, become increasingly important for our energy sustainability and environmental concerns. The search for improved electrocatalyst materials, which constitute the core of electrochemical energy conversion devices, has been typically dominated by the optimization of kinetic activity of catalysts and efficiency of whole cells. However, also the stability of the materials is highly important for a potential commercialization, if not even more important, and should at least always be considered in parallel. In this presentation I will demonstrate how such investigations are done on a fundamental level, and what can be learned from these studies for large scale applications. The focus will be on the recent methodological developments from our group, in particular the scanning flow cell (SFC) coupled to an ICP-MS for studying noble metal catalysts as used in low-temperature fuel cell electrochemical reactors.

O 76.5 Thu 17:45 H31

Quantitative void detection in thin platinum films by electrochemical means — •Michael Scheele, Damian Bürstel, and Detlef Diesing — Universität Duisburg - Essen, Fakultät für Chemie, Universitätsstrasse 2, D - 45141 Essen, Germany

In modern catalysis and energy conversion technologies thin metal films (10 - 100 nm) deposited on different substrates are widely used.

The wetting of the substrate by the metal during the deposition is crucial for the formation of voids and islands in the thin metal film. Due to a different catalytic behavior of small metal islands (nanoparticles) and different chemical behavior of the substrate (corrosion) the absence of voids and islands is desirable in most cases. A 10 nm thin platinum film is prepared on a substrate consisting of tantalum covered with an ultrathin tantalum oxide film (5 nm). Cyclovoltammetric experiments on the thin platinum film are carried out in sulfuric acid. Although platinum films show a quite good wetting behavior on the oxide, small fractions of uncovered substrate area can show up during preparation or in the electrochemical experiments. The high capacitance of the liquid-oxide-tantalum interface in the voids of the platinum film can be used to measure the charging current of the interface. Hereby the fraction of the substrate which is in contact with the electrolyte and not with the platinum can be estimated. The result indicates that this method is a good way for in-situ detection of uncovered area fractions down to 10^{-3} of an 10 nm thick platinum film during surface reactions in liquid media.

O 76.6 Thu 18:00 H31

Electrochemical activity of Ru(0001) electrodes modified by monolayer Au islands — •Tamara Husch, Otavio Brandao Alves, Albert K. Engstfeld, Sylvain Brimaud, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Bimetallic surfaces where a second metal covers part of a substrate bulk metal, exhibit unique catalytic properties which differ from those of the individual components and possibly also from those of a surface fully covered by a monolayer film of the second metal. The latter was demonstrated for PtML/Ru(0001) [1], where Pt islands act as catalyst for OH and H adsorption on the Ru(0001) substrate.

In this work we investigated whether similar effects can take place also on partly Au monolayer island covered Ru(0001) surfaces, or whether Au monolayers simply leads to blocking of the Ru(0001) surface. Submonolayer Au covered Ru(0001) surfaces were prepared by evaporation at room temperature under ultra high vacuum (UHV) conditions. After determination of the Au coverage by scanning tunneling microscopy (STM), the electrochemical properties of the Au/Ru bimetallic surface were characterized in an electrochemical flow cell attached to the UHV system. Surprisingly, the data show that the charge in the respective adsorption peaks is independent of the the Au coverage, and is always equivalent to a 0.2 ML Au coverage. Possible reasons leading to this unusual behavior are discussed.

[1] H. Hoster, B. Richter, and R.J. Behm, J. Phys. Chem B 108 (2004) 14780.

O 76.7 Thu 18:15 H31

Aligning electronic energy levels in electrochemical systems — •Mira Todorova and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

The relative position of a solid's band structure or an ion transition level with respect to the water energy levels is crucial for the understanding and quantification of electrochemical reactions at solid/liquid interfaces. In terms of electronic structure water has been shown to exhibit features similar to an amorphous semiconductor [1]. As such, it does not have well defined band edges, which makes the technique of aligning defect levels with respect to the band-edges, commonly used in semiconductor physics, not very practicable. Other alignment possibilities, which exploit the reduced sensitivity of an electrostatic potential or some deep level within the band-gap of a material with respect to the band-edge positions and their possible shift, upon changing the used exchange-correlations functional, have been discussed in the semiconductor literature. We explore the applicability of such techniques to electrochemical problems, by discussing the alignment of the electronic levels of ions in water. Utilising our findings and our recently developed method to identify the electrode potential and pH-value within an electrochemical system we explore the stability of ZnO surfaces as a function of environmental conditions.

[1] F. Williams, S.P. Varma, and S. Hillenius, J. Chem. Phys. 64, 1549 (1976).

O 76.8 Thu 18:30 H31

Structural Control of *ZnO* Thin Films Electrochemically Grown on Microstructured Electrodes — •Martina Stumpp, Christian Lupo, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Zinc oxide (ZnO) can be used as electrode material in dye sensitized solar cells and in microelectronic devices. Electrochemical deposition is an energy-efficient and economic processing method to obtain compact or porous crystalline thin films of ZnO. Microelectrodes were used as substrates for the electrodeposition of ZnO under pulsed galvanostatic conditions from aqueous zinc nitrate solutions. The ZnO growth was characterized by scanning electron microscopy and confocal laser microscopy. For current densities below the limiting current density, homogenous films were obtained, whereas for current densities greater than those limited by the diffusion of Zn^{2+} and NO_3^-, strongly dendritic structures were formed. The geometric distribution of the transport of the precursors from solution relative to the electrode surface and the subsequent formation of ZnO was discussed based on a model of a duplex diffusion layer. When polarizing only one of two sets of interdigitated microstuctured electrode bands a peculiar sequence of deposition either on the polarized electrode band and/or on the non-polarized electrode band was observed. An influence of convective diffusion was found to be the reason for such sequence.

O 76.9 Thu 18:45 H31

Electroless deposition of porous zinc oxide films on aluminium — •Stephanie Künze and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany.

Porous zinc oxide is discussed as an active semiconductor in dye-sensitized solar cells. Metal substrates are of interest to provide excellent conductivity and mechanical flexibility of cells. Metal substrates that are protected by an oxide layer in contact to air (passivated metal) can lead to cells containing even an iodide-containing electrolyte without the danger of corrosion. Aluminium can serve as such a metal substrate. Sheets of aluminium were pre-treated in highly-concentrated hydrochloric acid and subsequently in an alkaline zinc hydroxide solution (zincate stain). A coat of zincate was left on the aluminium surface. Porous zinc oxide films were prepared by electroless deposition on such pretreated planar aluminium substrates in the presence of the xanthene dye *EosinY* by two methods. Either a zinc-chloride solution saturated with oxygen or an aqueous solution of 0.1 M $Zn(NO_3)_2$ was used. The growth of zinc oxide was characterized by optical microscopy, scanning electron microscopy (SEM) and a stylus method to determine the layer thickness. The difference between the two forms of deposition is reported and a mechanism for this electroless deposition on aluminium is proposed and will be discussed. The influence of the amount of deposited zincate from the pre-treatment on the film thickness of the porous zinc oxide and the coverage of the metal surface is shown. In this context also results of an electroless deposition of porous zinc oxide on etched sheets of zinc was analyzed.

O 77: Electronic Structure and Spin-Orbit Interaction III

Time: Thursday 16:00–19:15 Location: H33

O 77.1 Thu 16:00 H33

Surface valence states and stoichiometry of non-superconducting and superconducting FeTe films — •Donald Telesca[1,2], Yuefeng Nie[1], Joseph Budnick[1], Barrett Wells[1], and Boris Sinkovic[1] — [1]University of Connecticut — [2]Air Force Research Laboratory

We report the surface electronic structure and stoichiometry of FeTe films following the incorporation of oxygen by three different methods: air exposure, dry oxygen exposure and low temperature oxygen annealing. X-ray photoemission experiments show that oxygen incorporation changes the initial valence state of Fe from 0 to mainly 3+. We also observe that the Te changes valence from initially 0 to mixed 0 and 4+. The rate of valence changes is seen to depend on the method of incorporation. In addition, it is observed that the surface of the FeTe films is left in a Te deficient state following any type of exposure to oxygen.

O 77.2 Thu 16:15 H33

Valence reconstruction at the surface of $LaCoO_3$ thin films studied by resonant x-ray reflectometry — •Jorge E. Hamann-Borrero[1,2], Abdullah Radi[2], Woo Seok Choi[3], Sebastian Macke[4], Ronny Sutarto[5], Feizhou He[5], George A. Sawatzky[2], Ho Nyung Lee[3], and Vladimir Hinkov[4] — [1]IFW-Dresden — [2]University of British Columbia, Vancouver, Canada — [3]Oak Ridge National Laboratory, Materials Science and Technology Division, USA. — [4]Max Planck-UBC Centre for Quantum Materials, Vancouver, Canada — [5]Canadian Light Source, Saskatoon, Canada

The structural and electronic properties of a set of $LaCoO_3$ (LCO) thin films with and without a $LaAlO_3$ capping layer are studied by means of resonant x-ray reflectometry (RXRR) and x-ray absorption spectroscopy. The data analysis was performed using an element and valence specific approach. Our observations show that, whereas the capped film shows homogeneous and undisturbed electronic properties throughout the whole LCO layer, the uncapped sample suffers a valence disproportionation where the film bulk has a Co^{3+} character and a Co^{2+} layer is formed at the film surface. The origin of this reconstruction and its relation to the magnetism is discussed. Our results demonstrate the power of RXRR in studying fine depth resolved electronic properties in thin films.

The work at Oak Rigde National Laboratory was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

O 77.3 Thu 16:30 H33

Direct band structure measurement of a buried two-dimensional electron gas: delta-doped Si(001) — Jill Miwa[1], Michelle Simmons[2], Philip Hofmann[1], and •Justin Wells[3] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNano), Aarhus University, 8000 Aarhus C, Denmark. — [2]Centre of Excellence for Quantum Computation and Communication Technology, School of Physics, University of New South Wales, Sydney, NSW 2052, Australia. — [3]Department of Physics, Norwegian University of Science and Technology (NTNU), N-7491 Trondheim, Norway

We directly measure the band structure of a buried two dimensional electron gas (2DEG) using angle resolved photoemission spectroscopy. The buried 2DEG forms 2 nm beneath the surface of p-type silicon, because of a dense delta-type layer of phosphorus n-type dopants which have been placed there. The position of the phosphorous layer is beyond the probing depth of the photoemission experiment but the observation of the 2DEG is nevertheless possible at certain photon energies where emission from the states is resonantly enhanced. This permits direct access to the band structure of the 2DEG and its temperature dependence. This material system has been chosen since delta-doped silicon is not only a testing ground for fundamental physics, but has demonstrated recent successes as a platform for the fabrication of atomic-scale devices for quantum computation applications. The measurement concept presented here should be applicable to a wide range of similarly important buried conductive layers.

O 77.4 Thu 16:45 H33

Angle-Resolved Photoemission on the Kondo Surface Alloy $CePd_7$ — •Mattia Mulazzi[1], Christoph Seibel[1], Holger Schwab[1], Kenya Shimada[2], Jiang Jiang[2], and Friedrich Reinert[1,3] — [1]Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — [2]Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan — [3]Karlsruhe Institute of Technology KIT, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

This films of the Cerium were evaporated on a Pd(001) substrate an further annealed to obtain a thin surface alloy layer of stoichiometry $CePd_7$, as observed by Auger spectroscopy. From LEED measurements it was possible to determine that the alloy has a $(\sqrt{5} \times \sqrt{5})R26.6^\circ$ reconstruction, commensurate to the Palladium substrate. Photon-energy dependent ARPES measurements crossing the 4d-4f resonance show the presence of a strong peak near the Fermi level, having actually two components, the actual Kondo peak at the Fermi level and the spin-orbit peak at 280 meV binding energy. Resonant and non-resonant Fermi surface maps shows large intensity variations of the Pd bands, when measured at the resonance, a sign of strong hybridization between the conduction and the 4f electrons. While previous work assigns the CePd7 to the class of intermediate valence systems, our work shows that it is actually a Kondo system, with a rather high Kondo temperature.

O 77.5 Thu 17:00 H33

Time-of-flight momentum microscopy with imaging spin filter — •Katerina Medjanik[1], Sergey Chernov[1], Hans-Joachim Elmers[1], Christian Tusche[2], Alexander Krasyuk[2], Jürgen Kirschner[2], and Gerd Schönhense[2] — [1]Institut für Physik, Univ. Mainz — [2]Max Planck-Institut für Mikrostrukturphysik, Halle

Momentum microscopy is a novel approach to study the electronic structure of surfaces using the cathode-lens technique, well-known from PEEM. Whereas a PEEM is optimized for best resolution in real space, momentum microscopy aims at an ultimate resolution in k-space (reciprocal space). Up to now, dispersive spectrometers have been used as energy filter [1]. In this contribution we present first results using time-of-flight (ToF) energy dispersion using a delayline detector, adopting concepts of ToF-PEEM [2]. By setting a ToF condition in the 3D (x,y,t) data sets, we define sections in k-space. We optimized the electron optical design such that for start energies up to 80eV the full half space above the sample surface (more than the first Brillouin zone) is imaged with high k-resolution. Using the imaging reflection-type spin filter [3,4], we were able to obtain spin resolution. The instrument allows highly efficient simultaneous spin filtering of many energy sections through momentum space.

Funded by BMBF (05K12UM2) and COMATT.

[1] B. Krömker et al., Rev. Sci. Instrum. 79 (2008) 053702.
[2] G. Schönhense et al., Surf. Sci. 480 (2001) 180.
[3] C. Tusche et al., APL 99 (2011) 032505.
[4] D. Kutnyakhov et al., submitted to Ultramicroscopy.

O 77.6 Thu 17:15 H33

Mapping Image Potential States on Graphene Nanoflakes — Fabian Craes[1], Sven Runte[1], Jürgen Klinkhammer[1], Marko Kralj[2], Thomas Michely[1], and •Carsten Busse[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut za fiziku, Zagreb, Croatia

Confinement effects of free electron like image potential states (IPSs) are observed in scanning tunneling spectroscopy (STS) on graphene nanoflakes on Ir(111) acting as potential wells. IPSs are unoccupied surface states energetically residing in an image charge potential between the Fermi and the vacuum level. They show a hydrogen-like spectrum perpendicular to the surface and form a two dimensional electron gas (2DEG) parallel to it.

We analyzed the IPSs by measuring local density of states (LDOS) point spectra as well as maps of the LDOS at selected energies. The spectra strongly depend on the size of the nanostructure as well as on the spatial position on top, indicating lateral confinement. The dominant contribution comes from a state other than the ground state due to parallel momentum transfer in the tunneling process. The confining potential can be tuned by intercalation.

O 77.7 Thu 17:30 H33

Development of a Megahertz high-harmonic light source for time-of-flight photoemission spectroscopy — •Cheng-Tien Chiang[1,2], Michael Huth[1], Alexander Blättermann[2], Jürgen Kirschner[1,2], and Wolf Widdra[2,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

We developed a tunable laboratory light source for time-of-flight photoemission spectroscopy using high-order harmonic generation at 4 MHz. The harmonics are driven by a commercial Ti-sapphire laser oscillator and generated in a tight-focusing geometry. Photons with energies beyond 20 eV are produced from an argon gas jet, and the intensity of harmonics can be significantly increased by using a xenon jet. With this light source, we demonstrate photoemission experiments at 4 MHz repetition rate on the well-known Cu(111) surface with a characteristic electronic structure [1].

[1] C.-T. Chiang, A. Blättermann, M. Huth, J. Kirschner, and W. Widdra, Appl. Phys. Lett. **101**, 071116 (2012)

O 77.8 Thu 17:45 H33

Femtosecond time-resolved photoemission on 1T-TaS_2 in the Mott-insulating state — •Isabella Avigo[1], Simon Freutel[1], Laurenz Rettig[1], Manuel Ligges[1], Lutz Kipp[2], Kai Rossnagel[2], and Uwe Bovensiepen[1] — [1](1)*Universitt Duisburg-Essen, D 47048 Duisburg — [2](2)*Christian-Albrechts-Universitt zu

Kiel, D 24118 Kiel

1T-TaS$_2$ is a quasi-two-dimensional transition metal dichalcogenide undergoing a metal-to-insulator transition below 180 K in which a charge density wave (CDW) coexists with a Mott insulating state. Of particular interest is the photoinduced melting of the Mott-Hubbard phase which drives the system in a crossover state [1,2] substantially different from the high temperature metallic state. Femtosecond time- and angle-resolved photoemission measurements were performed in the Mott-insulating phase at different pump fluences from 0.1 to 1 mJ/cm^2. We observe a population of states above the Fermi level (E_F) after pumping and a depletion and broadening of the Lower-Hubbard band (LHB) peak below E_F. From the analysis we carried out we clearly observe different relaxation dynamics of electron population above E_F, which decay in about 350 fs, and the intensity of the lower Hubbard band, recovering in about 900 fs. This points to a possible decoupling of populations above and below E_F and so to an at least non conventional metallic behavior of the photoinduced state.

We acknowledge support by the DFG through BO 1823/2, /4 and the EU under grant agreement 280555 within FP7. [1] Perfetti et al., NJP 10, 053019 (2008) [2] Dean et al., PRL 106, 016401 (2011)

O 77.9 Thu 18:00 H33

Electronic properties of Bi overlayers on Au(111) studied by low-temperature scanning tunneling spectroscopy — •Pin-Jui Hsu, Jeannette Kemmer, Jens Kügel, Tobias Mauerer, and Matthias Bode — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg, Germany

The Au(111) surface state is the paradigm of a Rashba-Bychkov system which—due to the large atomic spin-orbit coupling—exhibits the largest spin-splitting of all nobel metals [1]. Recent experiments have shown that the Rashba-splitting can be further enhanced by the adsorption of heavy adatoms [2]. In addition, complex spin textures have been predicted around isolated magnetic surface impurities [3]. In this contribution, we present scanning tunneling spectroscopy (STS) data of ultra-thin Bi films grown on Au(111). Our results indicate that the electronic structure strongly depends on the actual Bi coverage and surface structure. While the STS spectrum of the so-called (6×6)-structure observed at a coverage of about 0.5 atomic layers (AL) is almost featureless, the monolayer exhibits a strong peak in the differential conductance at $U = +2.3\,\mathrm{V}$, i.e. in the unoccupied sample states. For a local Bi coverage of 2 AL an asymmetric peak is observed at $U = +0.3\,\mathrm{V}$. We will discuss the potential origin of these electronic features and analyze if they are subject to Rashba-splitting.

[1] S. LaShell *et al.*, Phys. Rev. Lett. **77**, 3419 (1996).
[2] C. R. Ast *et al.*, Phys. Rev. Lett. **98**, 186807 (2007).
[3] S. Lounis, A. Bringer and S. Blügel, Phys. Rev. B **108**, 207202 (2012).

O 77.10 Thu 18:15 H33

Low-temperature superstructure of Au-induced atom chains on high-index silicon surfaces — •J. Aulbach[1], J. Schäfer[1], S.C. Erwin[2], S. Meyer[1], L. Dudy[1], B. Slomski[3], G. Landolt[3], H. Dil[3], and R. Claessen[1] — [1]Physikalisches Institut, Universität Würzburg, Germany — [2]Naval Research Laboratory, Washington DC, USA — [3]Paul Scherrer Institut, Villigen, Switzerland

Self-organized nanowires on high-index semiconductor substrates provide a versatile playground to scrutinize the low-temperature ground state of quasi-one-dimensional systems, such as a charge density wave (CDW) or a Tomonaga-Luttinger liquid. Here we report on Au nanowires on Si(553), where a structural model from density functional theory (DFT) [1] suggests strong spin-orbit coupling for the Au chains. Intriguingly, also antiferromagnetic spin order is proposed for the silicon structure along the terrace edges.

Scanning tunneling microscopy images of Au/Si(553) are found to be in astounding agreement with the structural model [1], including its periodicities. Moreover, tunneling spectroscopy measurements at low temperature indicate the absence of an energy gap. This does not support the picture of two coexisting CDWs, contrary to previous perception. Instead, the local density of states displays a distinctive structure which matches the spin-polarized Si step-edge state predicted by DFT. Finally, we briefly address the spin-orbit coupling in the Au bands using spin- and angle-resolved photoemission, providing direct evidence for a spin-splitting.

[1] S. C. Erwin and F. J. Himpsel, Nature Commun. **1**, 58 (2010).

O 77.11 Thu 18:30 H33

Probing current noise and topography in low-temperature scanning tunneling microscopes at sub-molecular resolution — •Markus Herz, Samuel Bouvron, Elizabeta Ćavar, Mikhail Fonin, and Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz

Noise studies have become an active field in mesoscopic physics because they reveal a variety of additional information about electronic correlations [1].

We probe the current noise in low-temperature scanning tunneling microscopes (STM). The measurement setup is modified for extracting the current noise and its spectral density without the necessity of double wiring and performing cross correlation [2] and without going to high frequency measurements [3].

We show simultaneous measurements of the tunneling current and its noise in a low-temperature STM [4] with a very high thermal, mechanical and electronic stability.

In first experiments, the Fano factor $F = 1$ is observed to be a sharp lower limit for the current noise scaling when imaging sub-molecular details of clusters produced on a metallic surface at a tunneling conductance of $\simeq 10^{-4} G_0$, and the noise power is not correlated with the topographic signal.

[1] Y. Blanter and M. Büttiker, Physics Report, 336 (2000)
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[3] R. Chen et al., Phys. Rev. B 85, 235455 (2012)
[4] C. Debuschewitz et al., J. Low. Temp. Phys. 147, 525 (2007)

O 77.12 Thu 18:45 H33

Long range charge transfer and electrostatics at a molecular heterojunction on a metal surface — •Patrick Amsalem[1], Jens Niederhausen[1], Andreas Wilke[1], Georg Heimel[1], Raphael Schlesinger[1], Stefani Winkler[1,2], Antje Vollmer[2], Jürgen P. Rabe[1], and Norbert Koch[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, BESSY II, Berlin, Germany

Understanding the energy level alignment (ELA) at organic heterostructures grown on conductive electrodes is of major importance for improving organic-based devices. In this work, the ELA at an electron acceptor molecule (C60) / organic spacer (alpha sexithiophene, 6T) / Ag(111) interface is investigated as a function of the 6T thickness (one and two monolayers) by means of photoelectron spectroscopy. The formation of an interface dipole with similar magnitude is found for the two studied systems. Valence band and core level measurements reveal that these interface dipoles result from an integer electron transfer from the metal towards the C60 molecules, through the 6T film [1, 2]. Consistently, the total amount of electrons transferred to the C60 film is found to decrease with increasing 6T thickness. Also, a potential drop within the 6T is observed. These findings are quantitatively addressed by electrostatic considerations to entangle the effect of dipole-dipole interactions and potential drops observed when the interface is formed. [1] P. Amsalem, et al., J. Phys. Chem. C 115, 17503 (2011) [2] J. Niederhausen et al., Phys. Rev. B 86, 081411 (R) (2012)

O 77.13 Thu 19:00 H33

Probing the electronic structure of salt solutions by resonant inelastic soft X-ray scattering — •Sankaranarayanan Nagarajan[1], Frank Meyer[2], Andreas Benkert[2,3], Marcus Bär[4,5], Regan Wilks[4], Wanli Yang[6], Friedrich Reinert[2], Clemens Heske[3,5], Lothar Weinhardt[3,5], and Michael Zharnikov[1] — [1]Angew. Phys. Chemie, Universität Heidelberg — [2]Exp. Phys. VII, Universität Würzburg — [3]Inst. for Photon Science and Synchr. Radiation, Karlsruhe Institute of Technology — [4]Sol. Energy Res., Helmholtz-Zentrum Berlin — [5]Dept. of Chemistry, University of Nevada, Las Vegas — [6]Advanced Light Source, Lawrence Berkeley National Laboratory

Salt addition to water induces changes in the hydrogen bond network. These changes can be monitored by Resonant Inelastic soft X-ray Scattering (RIXS) measurements, which provide information on the electronic structure of solids, liquids, gases, and (here) solutions. In this contribution, we present RIXS maps for the aqueous solutions of KCl and NaCl at different concentrations (from 1M to super-saturated solutions). Both resonant and non-resonant emission spectra derived from these maps are discussed in detail. We find changes in the positions and intensities of characteristic emission peaks as a function of salt concentration. The observed changes are rationalized in terms of structural perturbations induced by the salt, which, in turn, result in a change of the electronic structure.

O 78: Surface Dynamics I

Time: Thursday 16:00–19:15 Location: H42

O 78.1 Thu 16:00 H42

"Pick-up" mechanism in the scattering of hyperthermal N atoms off N-covered Ag(111) — •María Blanco-Rey[1], Estíbaliz Díaz[1], Gisela Bocan[2], Ludovic Martin-Gondre[1,3,4], Ricardo Díez-Muiño[1,3], Maite Alducin[1,3], and J. Iñaki Juaristi[1,3,5] — [1]Donostia International Physics Center, 20018 Donostia-San Sebastián, Spain — [2]CONICET and CNEA, 8400 S.C. de Bariloche, Argentina — [3]Centro de Física de Materiales, Centro Mixto CSIC-UPV/EHU, 20018 Donostia — [4]Institut des Sciences Moléculaires, CNRS UMR 5255 / Université Bordeaux I, 33405 Talence, France — [5]Dept. de Física de Materiales, Facultad de Químicas UPV/EHU, Ap. 1072, 20018 Donostia

An ab-initio 3D potential energy surface (PES) and classic molecular dynamics (MD) are used to study the reflection and adsorption dynamics of N atoms on N-covered Ag(111). We find that the surface N species modify the PES dramatically, adding corrugation and an attractive well above the adsorbed N, but MD shows that the scattered N angular distributions change little upon N adsorption, in agreement with molecular beams experiments. However, this level of theory fails to reproduce the experimental final-to-initial average energy ratios, $\langle E_f\rangle/\langle E_i\rangle$, at grazing angles. From a close examination of N sticking, we infer that gas N is likely to "pick-up" adsorbed N species to form N_2. This mechanism is active mainly at low energies. With this in mind, the experimental energy ratios are explained by the surface being partially cleaned as the experiment is being conducted. Simulations with a 6D PES support the "pick-up" process efficiency.

O 78.2 Thu 16:15 H42

Adsorption & dissociation of O_2 on Ag(100) – How much do we really know? — •Vanessa Bukas, Jörg Meyer, and Karsten Reuter — Technische Universität München, Germany

Despite the considerable attention it has received over the past decades, the adsorption of oxygen on silver surfaces remains elusive of an exact *microscopic* description [1,2]. Connecting and elucidating past results, the present theoretical work revisits the O_2-Ag(100) interaction from a density-functional theory (DFT) perspective – starting from the interpolated potential energy surface (PES) constructed by Alducin *et al.* within a recent dynamical study [2]. An extensive global search on this PES allows us to obtain all stable molecular adsorption configurations, corresponding vibrational modes as well as minimum energy paths leading from the former towards dissociation. While barriers of more than 1.2 eV do rationalize the low dissociative sticking probability [2], a conclusive assignment for the two species of adsorbed O_2 reported by Vattuone *et al.* [3] cannot be reached. Re-interpolation of the existing DFT data with a different technique [1] fails to account for potential shortcomings of the PES. Aiming to go beyond the limits of the previously employed pseudo potentials [2] in future dynamical studies, we will finally present first results of highly-accurate all-electron DFT calculations using the FHI-aims code [4].
[1] I. Goikoetxea *et al.*, New J. Phys. **14**, 013050 (2012).
[2] M. Alducin *et al.*, J. Chem. Phys. **129**, 224702 (2008).
[3] L. Vattuone *et al.*, Surf. Sci. **377**, 671 (1997).
[4] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).

O 78.3 Thu 16:30 H42

Non-adiabatic vibrational damping of O_2 on Ag(100): implications for light-enhanced heterogeneous catalysis? — •Simon P. Rittmeyer, Jörg Meyer, and Karsten Reuter — Technische Universität München, Germany

The dissociation of oxygen molecules is the rate limiting step in various surface catalyzed oxidation reactions like e.g. the industrially important epoxidation of ethylene. To this end, Linic and coworkers reported a remarkable improvement of the energy efficiency of cubic silver nano-catalysts upon irradiation with visible light, and attributed this to a selective enhancement of the O_2 dissociation step [1]. In their explanation, the non-adiabatic damping of the O-O stretch vibration of adsorbed O_2 plays a crucial role. As going beyond the Born-Oppenheimer approximation for the description of metal-adsorbate interactions is still an emerging field of first-principles based modeling, we will subject the latter to a perturbative treatment rooted in time-dependent density-functional theory, extending an ansatz originally developed to obtain electron-hole pair excitation spectra during adsorption processes (see e.g. [2] and references therein). Within this new approach, we will present estimates for the vibrational lifetime of O_2 adsorbed at various stable sites of the Ag(100) surface and critically discuss the implications for the model proposed by Linic and coworkers.
[1] P. Christopher, H. Xin, and S. Linic, Nature Chem. **3**, 467 (2011).
[2] J. Meyer and K. Reuter, New J. Phys. **13**, 085010 (2011).

O 78.4 Thu 16:45 H42

Surrogate Hamiltonian study of laser induced desorption of CO/NiO(100) and CO/TiO_2(110) — Erik Asplund and •Thorsten Klüner — Institut für Reine und Angewandte Chemie, Carl von Ossietzky Universität Oldenburg, Germany

In this study, microscopic models for electronic relaxation in femtosecond laser induced desorption experiments are presented. The surfaces in desorption experiments constitute environments for the molecules studied. Due to interactions between an adsorbed molecule and the surface, energy and phase exchange emerge. The photodesorption process consists of three steps: first the adsorbed molecule is excited by an external laser field, thereafter the relaxation process transfers energy to the surface and finally desorption. A theoretical investigation of laser induced desorption must hence treat all involved process, i.e. excitation, excited state dynamics and relaxation, on equal footing. This can be realized within the Surrogate Hamiltonian approach [1]. Furthermore, the Surrogate Hamiltonian method enables a microscopic description of excitation and relaxation process for open quantum systems. The Surrogate Hamiltonian approach is applied to electronic relaxation of CO adsorbed on NiO(100) and TiO_2(110). Ab initio electronic potential energy surfaces are combined with microscopic descriptions of the interactions between the adsorbed molecule with the surfaces in order to gain insight in the desorption mechanism. Furthermore, life times, desorption probabilities, and velocity distributions for the desorbing molecules are presented.
[1] R. Baer, and R. Kosloff, J. Chem. Phys. 106, 8862 (1997).

O 78.5 Thu 17:00 H42

The effect of vibrational amplitude on electronic energy dissipation via electron-hole pair-vibrational coupling — •Michael Grotemeyer and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

Time-dependent density functional calculations for vibrational highly excited HCl molecules in front of an Al(111)-surface have revealed a large non adiabatic energy dissipation. At the first glance this may appear to be in contrast to observations from scattering experiments for HCl/Au(111), which yield only a small energy dissipation into electron-hole pairs in case of low initial vibrational excitation of incoming molecule [1]. To explain this, we have studied the non adiabatic energy transfer by *ab initio* molecular dynamics simulations as a function of initial vibrational excitation energy, thereby filling the gap between experiment and previous calculations. We find a strong increase of dissipation with vibrational energy, which increases faster than linear and clearly deviates from the prediction by the linear friction ansatz. Results are further elucidated by means of a 1D tight binding model.
[1] I. Rahinov *et al.*, J. Chem. Phys. **129**. 214708 (2008).

O 78.6 Thu 17:15 H42

Calculation impossible – how far can we push electronic friction theory? — Francesco Nattino[1], •Jörg Meyer[2], Geert-Jan Kroes[1], and Karsten Reuter[2] — [1]Leiden University, Netherlands — [2]Technische Universität München, Germany

One of the prevailing challenges for modeling the motion of molecules on metal surfaces is to go beyond the Born-Oppenheimer approximation in order to account for the potential influence of the continuum of electron-hole pair excitations [1]. Amongst other approaches rooted in time-dependent density functional theory [2], electronic friction theory has the compelling advantage of being a computationally convenient enhancement of classical dynamics for the nuclei – if friction coefficients can be easily and accurately calculated. Along those lines, results obtained within the local density friction approximation (LDFA) applied independently for each atom of a diatomic have fueled a controversial discussion only recently [3]. In an attempt to disentangle both the LDFA and independent atom approximation for the friction coefficients, we will illustrate a new idea of how to obtain the full-dimensional molecular friction tensor, which is easy to combine with the mapping of high-dimensional potential energy surfaces. First results will be presented using H_2 on Cu(111) as a showcase.

[1] G.-J. Kroes, Science **321**, 794 (2008).
[2] J. Meyer and K. Reuter, New J. Phys. **13**, 085010 (2011).
[3] J. I. Juaristi *et al.*, Phys. Rev. Lett. **100**, 116102 (2008), A. C. Luntz *et al.*, *ibid.* **102**, 109601 (2009), J. I. Juaristi *et al.*, *ibid.* **102**, 109602 (2009).

O 78.7 Thu 17:30 H42

Helium-3 spin echo measurements and simulation of pentacene on pentacene surface diffusion

— •Paul Rotter[1], Antonia Morherr[2], Barbara Lechner[3], David Chisnall[3], Andrew Jardine[3], John Ellis[3], William Allison[3], Bruno Eckhardt[1], and Gregor Witte[2] — [1]Komplexe Systeme, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Molekulare Festkörperphysik, Philipps-Universität Marburg, 35032 Marburg, Germany — [3]Cavendish Laboratory, Cambridge, CB3 0HE, UK

With the Helium-3 spin echo technique (3HeSE) surface diffusion processes can be directly observed at their characteristic length scales (nm) and time scales (ps). While previous experiments focused on small adsorbates and metal surfaces, we advance to comparatively large organic diffusing adsorbates and organic surfaces. In this study a coplanar monolayer of pentacene chemisorped on Cu(110) was used as a well characterized organic surface on which isolated pentacene molecules diffuse. 3HeSE measurements which contain a complete statistical description of the adsorbate motion were carried out for different azimuthal directions of the surface. To extract the different processes that contribute to the diffusion, we use molecular dynamics simulations to compare to and reproduce key features of the experimental results. The potential energy surfaces needed for those simulations are constructed via molecular mechanics.

O 78.8 Thu 17:45 H42

Spatial dependence of vibronic excitations

— •Niko Pavliček[1], Ingmar Swart[2], Judith Niedenführ[3], Gerhard Meyer[4], and Jascha Repp[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, the Netherlands — [3]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Germany — [4]IBM Research–Zurich, 8803 Rüschlikon, Switzerland

In organic and molecular electronics the electrons are much more spatially confined as compared to inorganic semiconductors, leading to a much stronger electron-vibron (e-ν) coupling. e-ν coupling therefore gives rise to substantial dissipation in such systems. When an electron tunnels into a given molecule (electron attachment), the nuclei will relax giving rise to the so-called reorganization energy, a process that is usually treated in the Franck-Condon picture.

Here, we show that even for an effective single-level system, the spatial position of the electron injection as well as the wave function strongly affect the e-ν coupling strength. These findings can be rationalized by symmetry arguments, thereby shedding new light onto e-ν coupling in organic and molecular electronics.

To this end, we performed low temperature scanning tunneling spectroscopy experiments on individual pentacene molecules adsorbed on ultrathin insulating films.

O 78.9 Thu 18:00 H42

Deposition of model chains on surfaces: anomalous relation between flux and stability

— •Pritam Kumar Jana[1] and Andreas Heuer[2] — [1]Westfälische Wilhelms-Universität Münster, Institut für Physikalische Chemie, Corrensstr. 28/30, 48149 Münster, Germany — [2]Westfälische Wilhelms-Universität Münster, Institut für Physikalische Chemie, Corrensstr. 28/30, 48149 Münster, Germany

We have investigated model chains which are deposited on the surface with a fixed flux via Monte Carlo simulations. They are supposed to mimic stiff lipophilic chains with a head group and tail groups, reflecting an alkyl chain. After some subsequent fixed simulation time we determine the final energy as a function of flux and temperature. Surprisingly we observe that in some range of temperature and flux the final energy increases with decreasing flux. The physical origin of this counterintuitive observation is elucidated. In contrast, when we are performing equivalent cooling experiments no such anomaly is observed. Furthermore, it is discussed whether flux experiments produce configurations with lower energies as compared to cooling experiments. These results are related to recent experiments by the Ediger group[1] where very stable configurations of glass-forming systems have been generated via flux experiments.

Reference:

1. K. L. Kearns, S. F. Swallen, M. D. Ediger, T. Wu, Y. Sun, and L. Yu, J. Phys. Chem. B 112, 4934 (2008).

O 78.10 Thu 18:15 H42

Laser triggered desorption of noble gases from tungsten tips studied by laser-assisted field ion microscopy (FIM)

— •Armin Feist, Sascha Schäfer, Carsten Nowak, and Claus Ropers — Materials Physics Institute and Courant Research Centre, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Field ion microscopy (FIM) is the oldest experimental technique to characterize surface structures of sharp tips on an atomic level. In the related technique of laser-assisted atom probe tomography (APT), ultrashort laser pulses are used for layer-by-layer surface atom removal and the reconstruction of three-dimensional structures. While being a powerful method, the actual dynamics of surface processes cannot be revealed in this approach, and the full capabilities of ultrafast spectroscopy are usually not exploited. Combining FIM with ultrafast pump-probe techniques carries the potential to study surface dynamics with atomic precision, provided that image gas desorption can be induced in a controlled way within ultrafast time intervals. In order to explore such concepts, using tunable femtosecond laser pulses, we study the photo-induced desorption of noble gas atoms from sharp tungsten tips by time-of-flight spectroscopy. The ionization rate is characterized as a function of static electric field, temperature, incident wavelength and laser fluence for various gases (He, Ne and Ar), yielding insights into the respective microscopic desorption mechanisms. We find highly stable and repeatable desorption rates under quasi-steady state conditions. Two-pulse correlation measurements allow for a time-resolved analysis and the disentanglement of thermal from nonthermal effects.

O 78.11 Thu 18:30 H42

Turning on and off the rotational oscillation of a single porphine molecule by molecular charge state

— •Shichao Yan[1,2], Zijing Ding[1], Nan Xie[1], Huiqi Gong[1], Yang Guo[1], Xinyan Shan[1], Sheng Meng[1], and Xinghua Lu[1] — [1]Beijing National Laboratory for Condensed-Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — [2]Max Planck Research Group-Dynamics of Nanoelectronic Systems, Center for Free-Electron Laser Science, Hamburg

The rotation dynamics of single magnesium porphine (MgP) molecules on ultrathin NaCl bilayer is investigated with low temperature scanning tunneling microscopy (STM) and density functional theory (DFT) calculations. It is observed that the rotational oscillation between two stable orientations can be turned on and off by the molecular charge state, which can be manipulated with the tunneling electrons. The features of the charge states and the mechanism of molecular rotational on/off state control are revealed at the atomic scale. The dependence of molecular orientation switching rate on the tunneling electron energy and the current density illustrates the underlying resonant tunneling excitation and single electron process. The drive and control of molecular motion with tunneling electrons demonstrated in this study suggests a novel approach towards electronically controlled molecular rotors and motors.

O 78.12 Thu 18:45 H42

Surface Dynamics of Sb(111) Measured with Helium Atom Scattering

— •Michael Mayrhofer-Reinhartshuber, Anton Tamtögl, Patrick Kraus, Markus Polanz, and Wolfgang E. Ernst — Institute of Experimental Physics, Graz University of Technology, Graz, Austria

Especially due to its appearance in a group of compounds belonging to the lately discovered class of topological insulators, the semimetal antimony (Sb) is an interesting candidate for investigations of its surface properties. Recently the surface phonon dispersion curve of Sb(111) was calculated using density functional perturbation theory [1], but there has been a lack of experimental data.

First Helium Atom Scattering measurements of the Sb(111) surface were performed by our group, showing sharp diffraction peaks in good agreement with the already known surface structure. The analysis of resonance features in our spectra revealed three bound states. The best fit helium-surface interaction potential shows a pure van der Waals character. By using time-of-flight measurements the surface phonon dispersion was obtained. The acoustic modes are in good agreement with ab-initio calculations. In analogy to measurements on Bi(111) [2, 3], vibrations of the electron corrugation originating in displacements of atoms in the second bilayer were detectable. These subsurface modes can only be observed by HAS because of the electron phonon coupling.

[1] D. Campi et al., Phys. Rev. B. 86 (2012) 075446

[2] M. Mayrhofer-Reinhartshuber et al., JPCM 24 (2012) 104008

[3] T. Tamtögl et al., Phys. Rev. B., submitted 2012

O 78.13 Thu 19:00 H42

Switching dynamics in laser-driven phase change materials probed by time-resolved X-ray diffraction — •Florian Quirin[1], Azize Koc[1], Matthieu Nicoul[1], Peter Zalden[2], Jan Siegel[3], Mariano Trigo[4], Pererik Andreasson[5], Henrik Enquist[5], Michael Shu[4], Tommaso Pardini[6], Matthieu Chollet[7], Diling Zhu[7], Henrik Lemke[7], Aaron Lindenberg[4], David Reis[4], Jörgen Larsson[5], Stefan Hau-Riege[6], Matthias Wuttig[2], and Klaus Sokolowski-Tinten[1] — [1]University of Duisburg-Essen, Germany — [2]RWTH Aachen, Germany — [3]CSIC, Madrid, Spain — [4]PULSE@SLAC, USA — [5]Lund University, Sweden — [6]LLNL, Livermore, USA — [7]SLAC, Menlo Park USA

Phase change materials (PCMs) exhibit rapid and reversible phase transitions between an amorphous and a crystalline state, which can be triggered by short light pulses. Since the structural changes are associated with large differences in the optical properties of the two phases, PCMs are widely used in rewritable optical data storage technology (e.g. RW-DVDs). We have used time-resolved X-ray scattering at the Linear Coherent Light Source (LCLS) to directly probe the structural dynamics in PCMs (GeSb, GST, AIST) after fs laser irradiation over an extended time range from fs to μs, thus obtaining complete information on the phase transition dynamics. All transitions (amorphous-to-crystalline and vice versa) seem to involve melting of the material. Depending on the excitation strength melting can occur on a sub-ps time-scale as a non-thermal process. However, it takes ns up to μs for the material to resolidify and to reach the final state.

O 79: Oxide Surfaces III

Time: Thursday 16:00–18:30 Location: H45

O 79.1 Thu 16:00 H45

Identification of the surface phonons of $BaTiO_3(100)$ and ultrathin films of $BaTiO_3$ on metal substrates — •Florian Schumann[1], Klaus Meinel[1], Andreas Trützschler[1], Konrad Gillmeister[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle

Phonons and their softening are key elements for the understanding of the long range coupling in ferroelectric and multiferroic materials which causes, e.g., the paraelectric to ferroelectric phase transition. In thin films these ferroelectric properties are often controlled by strain from the underlying substrate or heterostructure. Here we study the surface phonons of a $BaTiO_3(100)$ single-crystal and of $BaTiO_3(100)$ thin films grown by MBE and magnetron sputtering on Pt(100) and Au(100). HREELS spectra for all cases are dominated by three well-developed phonon peaks at about 220, 460, and 650 cm^{-1}. The latter two are identified as A(TO) surface modes. For thin films on Pt(100) and on Au(100) shifts of the surface phonons are observed due to misfit strain of +2% and -2%, respectively, as compared to the single crystal. Changes of the vibrational properties due to film thickness and temperature will be discussed.

O 79.2 Thu 16:15 H45

In-situ PFM characterization of ferroelectric domain properties of epitaxially $BaTiO_3(100)$ ultrathin films on Pt(100) — •Andreas Trützschler[1], Maik Christl[1], Stefan Förster[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle

The combination of ferroelectric and ferromagnetic oxides in heterostructures can lead to new multiferroic materials. For this concept the surface and interface properties are crucial and might deviate from bulk properties [1]. So far nearly all ferroelectric characterizations for thin films of the ferroelectric $BaTiO_3$ have been carried out ex-situ under ambient conditions [2]. In contrast, we present here an in-situ PFM characterization of UHV-prepared $BaTiO_3(100)$ thin films which have been grown on Pt(100). Due to the lattice mismatch the film is compressed by 2 % which causes a c-domain configuration [3]. The resulting domain pattern has been locally controlled by applying a DC voltage via the AFM tip. For ultrathin films the ferroelectric properties, especially the local hysteresis curve, indicate an inequivalence of outward and inward polarized c domains.

[1] A. Höfer et al., PRL 108, 087602 (2012).

[2] A. Gruverman et al., Nano Letters 9, 3539 (2009).

[3] S. Förster et al., JCP 135, 104701 (2011).

O 79.3 Thu 16:30 H45

Stress measurements during growth of $BaTiO_3$ and $SrTiO_3$ films on Pt(001) — •Jörg Premper, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

The measurement of film stress by the cantilever deflection technique is well established to study the correlation between stress and physical properties with monolayer sensitivity for metal-on-metal epitaxy [1]. The epitaxy of functional oxides such as $BaTiO_3$ (BTO) and $SrTiO_3$ (STO) requires experimental conditions, which deviate sharply [2] from that of metal epitaxy. A high substrate temperature (700°C) and a substantial oxygen partial pressure (1×10^{-4} mbar) during film growth by pulsed laser deposition (PLD) are necessary for good epitaxial growth, but challenging for stress measurements in view of thermal drift and oxidation of the sample holder. An experimental setup is described, which allows quantitive stress measurements under these conditions. We present the first stress measurements during PLD of epitaxial BTO and STO monolayers on Pt(001). We find that the deposition of 20 ML BTO on Pt(001) (misfit = -1.9%) leads to a compressive film stress of -4.2 GPa, whereas the deposition of STO (misfit = +0.4%) induces a tensile stress of +1.2 GPa. The measured film stress is for both systems in good agreement with calculated misfit-induced stress.

[1] J. Premper, D. Sander, and J. Kirschner, Rev. Sci. Instr. **83**, 073904 (2012)

[2] J. Schwarzkopf, R. Fornari, Prog. Cryst. Growth Charact. **52**, 159-212 (2006)

O 79.4 Thu 16:45 H45

Density functional theory study of the $SrTiO_3$+TiO_x (110) surface — •Marcel Hieckel[1], Florian Mittendorfer[1], Josef Redinger[1], Raimund Podloucky[2], Michael Weinert[3], and Laurence Marks[4] — [1]Institute of Applied Physics, Vienna University of Technology, Austria — [2]Institute for Physical Chemistry, University of Vienna, Austria — [3]Department of Physics, University of Wisconsin - Milwaukee, USA — [4]Department of Materials Science and Engineering, Northwestern University, USA

Surfaces of oxide perovskites are of interest because of their intriguing physical properties. In partiuclar, growing transition metal oxid layers is of interest to design new catalysists.

We present results of density functional theory (DFT) calculations for the adsorption of TiO_x layers on $SrTiO_3$ (110) which were performed by VASP. For the exchange-correlation functional the generalized gradient approximation of Perdew-Burke-Ernzerhof [1] was used.

The thermodynamically stable surface structures for varying TiO_x compositions were studied to determine the phase diagram as a function of the TiO_x concentration by making use of the chemical potentials of oxygen and titanium. Scanning tunneling microscopy (STM) images are simulated within the Tersoff-Hamann approximation [2] which are compared to very recent low temperature STM experiments. Work supported by the Austrian FWF, project Nr. F4511-N16.

[1] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865(1966). [2] J. Tersoff and D. R. Hamann, Phys. Rev. B 31, 805 (1985).

O 79.5 Thu 17:00 H45

Post deposition annealing of ceria *films on Si(111) — •Henrik

Wilkens[1], Robert Oelke[1], Olga Schuckmann[1], Reinhard Olbrich[1], Marvin H. Zoellner[2], Thomas Schroeder[2], Michael Reichling[1], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

A 250 nm cub-CeO$_2$(111) film grown on hex-Pr$_2$O$_3$/Si(111) is annealed under UHV conditions. Atomic force microscopy (AFM) and spot profile low energy electron diffraction (SPA-LEED) were used to resolve the surface morphology. The chemical composition was studied by photoelectron spectroscopy (XPS). In addition, the changes of the bulk structure were probed by in-situ x-ray diffraction (XRD) measurements.

The surface exhibit triangular shaped facets as shown by AFM which vanish at higher temperatures. Moreover, several superstructures appear in the LEED pattern due to ordered oxygen vacancy formation. Also the XPS data shows that the surface reduces continuously at higher annealing temperatures.

The XRD measurements reveal that not the whole film is reduced since a diffraction signal of cub-CeO$_2$(111) is still visible at elevated temperatures. Furthermore, it is shown that above a critical temperature the hex-Pr(0001) buffer layer is destroyed and silicon diffuses into the ceria film.

O 79.6 Thu 17:15 H45

Characterization of thin cerium oxide films on Cl/Si(111) studied by GIXRD and XPS — •Jan Höcker[1], Björn Kaemena[1], Florian Bertram[2], Jan Ingo Flege[1], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen — [2]Hamburger Synchrotronstrahlungslabor am Deutschen Elektronensynchrotron, 22607 Hamburg

Cerium oxide is of strong interest in today's research because of its catalytic properties as well as its potential application in microelectronics, e.g., as an epitaxial high-k gate oxide on Si. As known from previous studies of ultrathin cerium oxide films on Si(111) (cf. Flege et al., PRB **84**, 2011), Cl-passivation facilitates epitaxial growth of the sesquioxide Ce$_2$O$_3$ phase and suppresses amorphous interface formation.

We have investigated the structural and chemical composition of 3 - 18 nm thin cerium oxide films grown by reactive MBE on either clean or Cl-passivated Si(111) by ex-situ grazing-incidence x-ray diffraction (GIXRD) and x-ray photoelectron spectroscopy (XPS). Only for Cl-passivated substrates reciprocal space mapping reveals well ordered oxide films. Capped samples show a dioxide fluorite (Ce^{4+}) as well as a sesquioxide bixbyite (Ce^{3+}) phase in contrast to uncapped samples, which only show a dioxide phase. XPS confirms a larger Ce^{4+} proportion for passivated substrates after exposure to ambient conditions whereas a mixture of Ce^{3+} and Ce^{4+} in the non-passivated case is observable. We conclude that only on passivated Si(111) a metastable Ce$_2$O$_3$ film crystallizes, which is converted into a well ordered dioxide phase under ambient conditions.

O 79.7 Thu 17:30 H45

Preparation and characterization of electrochemically deposited cerium oxide films — •Marc Sauerbrey[1], Jan Ingo Flege[1], Robert Rettew[2], Faisal Alamgir[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany — [2]School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, USA

Cerium oxide has been under intensive investigation over the last decades due to its interesting structural (oxygen storage capacity) and electronic properties (unfilled 4f shell). These properties result in a pronounced chemical reactivity as well as an enhancing effect on the reactivity of catalytically active metals like Pt, Au, and Rh.

In contrast to ultrahigh-vacuum methods, electrochemical preparation approaches are scalable, less complex and less expensive and thus are a promising alternative for industrial production purposes. In this contribution we present our results on the electrochemical growth and modification of cerium oxide films on Au and high-surface-area carbon substrates. A combined XPS (X-ray photoelectron spectroscopy) and SEM (scanning electron microscopy) analysis of as-prepared films shows predominantly fully oxidized cerium oxide with a rough morphology. Based on the analysis of Ce3d and O1s XPS data, annealing in oxygen atmosphere converts cerium oxide in predominantly CeO$_2$ (ceria). Furthermore, the influence of the ceria support on the oxidation state of post-deposited Pt will be discussed. First results indicate a ceria-promoted platinum oxidation, leading to the formation of PtO$_2$ particles.

O 79.8 Thu 17:45 H45

Probing Surface and Bulk Phonons in Nickel Oxide — •Srijan Kumar Saha[1], Oleg Brovko[1], Sebastian Polzin[2], Krassimir Kostov[2], Florian Schumann[2], Wolf Widdra[2], and Valeri Stepanyuk[1] — [1]Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle/Saale, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik FG Oberflächen- und Grenzflächenphysik, Von-Danckelmann-Platz 3, 06120 Halle/Saale

Using first-principles density-functional theory, we determine the vibrational properties of bulk NiO and its N-layer films; and compare our results with experiments performed by high-resolution electron energy loss spectroscopy (HREELS) on NiO(100) films on Ag(100). Because of the strong Coulomb interaction between the 3d electrons on the transition-metal ion, here we apply the DFT+U approach for this oxide, known as a model system of Mott or charge-transfer insulators. We find that the highest frequency surface optical phonon mode is highly dispersive and exhibits a huge blueshift as a function of number of layers in the film. The underlying physics of our main results will be discussed together with the pictorial representation of the phonon modes.

O 79.9 Thu 18:00 H45

Is the BaTiO$_3$ (001)-(2x1) reconstruction magnetic ? — •Holger. L. Meyerheim[1], A. Ernst[1], K. Mohseni[1], I.V. Maznichenko[2], S. Ostanin[1], F. Klimenta[1], N. Jedrecy[3], W. Feng[1], I. Mertig[2], R. Felici[4], and J. Kirschner[1] — [1]Max-Planck-Institut f. Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Institut f. Physik, Martin-Luther-Univ. Halle-Wittenberg, D-06099 Halle, Germany — [3]Institut des Nano Sciences de Paris, UPMC-Sorbonne Univ., CNRS-UMR7588, 75005 Paris, France — [4]ESRF, B. P. 220, F-38043 Grenoble Cedex, France

Though BaTiO$_3$ is the prototype perovskite type ferroelectric and its (2x1) reconstruction has been observed more than 30 years ago [1] no detailed analysis of its atomic geometry has been reported so far. We have carried out a surface x-ray diffraction analysis of the BTO(001)-(2×1) reconstructed surface [2]. While the crystal is terminated by two TiO$_2$ layers similarly to SrTiO$_3$(001)-(2×1) [3], we find that one Ti-atom of the top TiO$_2$ layer resides in a tetragonal pyramidal oxygen environment. Ab initio calculations based on this structure model suggest that the surface is metallic and magnetic involving local magnetic moments up to $2\mu_B$ in magnitude located at surface Ti and O atoms.

References: [1] R. Courths, Phys. Status Solidi B 100, 135 (1980) [2] H. L. Meyerheim, A. Ernst, K. Mohseni, I. V. Maznichenko, S. Ostanin, F. Klimenta, N. Jedrecy, W. Feng, I. Mertig, R. Felici,, and J. Kirchner, Phys. Rev. Lett. 108, 215502 (2012) [3] N. Erdman, K.R. Poeppelmeier, M. Asta et al., Nature 419, 55 (2002)

O 79.10 Thu 18:15 H45

An Atomic-Force-Microscopy study of Cu$_2$N on Cu(100) — •Maximilian Schneiderbauer, Matthias Emmrich, and Franz J. Giessibl — Regensburg University, Department of Physics, Regensburg, Germany

Recently Loth et al. [1] showed a new approach to push the spatial size of stored bits to the atomic scale. They tailored a switchable antiferromagnetic nanostructure made of a (2x6) Fe atom array exhibiting large magnetic anisotropy. To magnetically decouple this stand-alone spin structure from the conducting Cu substrate they used Cu$_2$N.

Thorough Scanning-Tunneling-Microscopy (STM) studies revealed the incommensurability of Cu$_2$N monolayer islands on Cu(100) [2, 3]. Although Cu$_2$N was as of yet just used in (spin polarized) STM experiments it is a promising candidate for magnetic sensitive Atomic-Force-Microscopy measurements. We have shown the qPlus setup capable of imaging magnetic domains [4] and, more recently, of detecting spin contrast [5]. Therefore we are currently studying Cu$_2$N on Cu(100) for future work on magnetic exchange force microscopy. In this contribution we show recent results from our home-built low-temperature qPlus setup.

[1] S. Loth et al Science 335, 196-199 (2012).
[2] F.M. Leibsle et al Surf. Sci. 317, 309-320 (1994).
[3] T. Choi et al Phys. Rev. B 78, 035430 (2008).
[4] M. Schneiderbauer et al Beilstein J. Nanotechnol. 3, 174-178 (2012).
[5] F. Pielmeier et al submitted.

O 80: Annual General Meeting of the Surface Science Division

Time: Thursday 19:30–20:00 Location: H36

30 min. General Meeting

O 81: Post-Deadline Session

Time: Thursday 20:00–21:00 Location: H36

Contributed Post-Deadline talks

O 82: Invited Talk (Richard Berndt)

Time: Friday 9:30–10:15 Location: H36

Invited Talk O 82.1 Fri 9:30 H36

Plasmons, forces and currents in atomic and molecular contacts — •Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel

The electron transport through single atoms, molecules and molecule–molecule contacts is investigated with low-temperature scanning probe microscopy. In the experiments, which aim at maximizing the control over the junction properties, the conductance, the acting force and the emission of photons are probed. The talk will address the role of molecular structure and bonding as well as localized plasmons and quantum noise properties.

O 83: Symposium Frontiers of Electronic Structure Theory: Discovery of Novel Functional Materials (SYES, jointly with DS, HL, MA, MM and TT)

Time: Friday 9:30–12:00 Location: H1

Invited Talk O 83.1 Fri 9:30 H1

Molecular dynamics simulation of nucleation and growth of crystals from solution — •Michele Parrinello — Department of Chemistry and Applied Biosciences, ETH Zurich and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, Lugano, Switzerland

Nucleation and growth of crystals from solution is a phenomenon of great practical relevance. Yet its study is rather challenging both experimentally and theoretically. Computer simulations could be of great help however they are rather difficult. To this effect we have developed a number of methods that can help overcoming many of the difficulties. We shall present results on the growth of urea from aqueous solutions in the presence and the absence of additives. We show how additives in particular biuret can control the shape of the growing crystal. We also show how the nucleation from saturated water solution of the humble NaCl hides some remarkable surprises.

Invited Talk O 83.2 Fri 10:00 H1

Describing, understanding, and discovering hybrid materials from first principles — •Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Germany

Hybrid materials are most exciting as one can expect new properties arising at the interface, which are absent in either of the building blocks. At the same time, they represent challenging cases for electronic-structure theory. Methods that turned out useful for describing one side may not be applicable for the other one, and they are likely to fail for the interfaces. For selected examples of organic/inorganic hybrid interfaces for light emitting applications and photovoltaics, I will present structural properties, electronic bands, and optical excitation spectra as obtained from density-functional theory and many-body perturbation theory. They will highlight which properties can be reliably computed for such materials. It needs to be also discussed, however, what is missing to reach predictive power on a quantitative level and, thus, open a perspective towards the discovery of new materials.

Invited Talk O 83.3 Fri 10:30 H1

Mapping the Electronic Structure Landscape for Materials Discovery — •Krishna Rajan — Iowa State University, Ames IA, USA

Normally, structure*property relationships are guided by defined functional relationships (e.g. electronic structure calculations to define energy landscapes associated with crystal chemistry) and many groups have developed powerful and extensive computational strategies based on electronic structure calculations to search large virtual chemical spaces to identify potentially new compounds. However, we propose a different approach to establish such a structure* property relationships where we do not assume any specific formulation linking structure with property. Rather, we take a data-driven approach where we seek to establish structure*property relationships by identifying patterns in a large and diverse array of data associated with both crystallographic and electronic structure calculations. By coupling statistical learning methods to map such high dimensional data in lower dimensions, we show how we can discover new materials chemistries with targeted properties.

Invited Talk O 83.4 Fri 11:00 H1

New ferroelectrics and antiferroelectrics by design — •Karin Rabe — Rutgers, the State University of New Jersey, USA

I will describe our work on the design and discovery of new classes of ferroelectric and antiferroelectric materials using a combined crystallographic database / first principles approach. For ferroelectrics, using the design principle that any polar structure type can have ferroelectric representatives if the barrier to switching is lowered by appropriate chemical variation, we have recently identified a new family of ferroelectrics in the intermetallic LiGaGe structure type. For antiferroelectrics, we used a design principle based on the close relationship between ferroelectrics and antiferroelectrics to identify a previously unrecognized class of antiferroelectrics, related to the LiGaGe-type ferroelectrics, in the MgSrSi structure type. The discovery of new classes of antiferroelectrics is expected to open the way to increased recognition and application of antiferroelectrics as functional materials.

Invited Talk O 83.5 Fri 11:30 H1

The Materials Project: The design of materials using high-throughput ab initio computations — •Gerbrand Ceder — Massachusetts Institute of Technology, Cambridge MA, USA

The need for novel materials is the technological Achilles Heel of our strategy to address the energy problem facing the world. The ”Materials (Genome) Project*, has as its objective to use high-throughput first principles computations on an unparalleled scale to discover new materials for energy technologies. Only computationally driven materials design can deal with the scale and urgency of the materials discovery problem. I will show how several key problems such as crystal structure prediction and accuracy limitations of standard Density Functional Theory methods have been overcome to perform reliable, large scale materials searching. In addition, once large data sets are developed, machine learning can be used to extract insight and design rules. I will show successful examples of high-throughput calculations in the field of lithium batteries, and show several new materials that have been discovered. In addition, I will discuss the public release version of the Materials Project which is making large quantities of computed data freely available to the materials community. (www.materialsproject.org).

O 84: Photovoltaics (jointly with CPP, DS and HL)

Time: Friday 9:15–13:45 Location: H2

O 84.1 Fri 9:15 H2

Simulation of TRPL on thin film solar cells — •Matthias Maiberg, Maria Gaudig, and Roland Scheer — Institute of Physics, Martin-Luther-University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06406 Halle, Germany

In the recent years time-resolved photoluminescence (short: TRPL) on semiconductor devices has been established as a non-destructive, non-invasive, contactless characterization method. The decay of the signal has not been fully understood yet. Therefore we studied TRPL on semiconductor layers and thin film solar cells by simulation with Synopsys TCAD. At first we investigated the influence of excitation, diffusion, photon recycling, bulk-defects and defects at the contacts, as well as space charge and potential fluctuations on the PL-decay separately by quasi-onedimensional simulations of absorber layers and thin film solar cells. We also studied the influence of grain boundaries, since materials like $\mathrm{Cu(In,Ga)Se_2}$ and $\mathrm{Cu_2ZnSnSe_4}$ are in general polycrystalline. We show, that the samples can be characterized by excitation dependent measurements in the open circuit case. We can explain some effects found in photoluminescence experiments, like a decrease of the lifetime with an increasing excitation, a maximum lifetime due to saturated bulk-defects, and a lifetime of more than $10\mu s$ in case of charge separation due to the electric field in the space charge region.

O 84.2 Fri 9:30 H2

3D reciprocal space imaging of individual $\mathrm{Cu(In,Ga)Se_2}$ nanocrystallites inside a thin film solar cell — •Taras Slobodskyy[1], Anatoliy Slobodskyy[2], Boris Landgraff[1], Christian Heyn[1], and Wolfgang Hansen[1] — [1]Institute for Applied Physics, University of Hamburg, Jungiusstraße 11, D-20355 Hamburg, Germany — [2]Karlsruhe Institute of Technology (KIT), Light Technology Institute (LTI), Kaiserstraße 12, 76131 Karlsruhe, Germany

In this contribution we will present results of an investigation of strain distributions inside of individual $\mathrm{Cu(In,Ga)Se_2}$ nanocyrstallites located inside a solar cell absorber layer. The strain is imaged using synchrotron radiation.

We find that the investigated crystallites are non homogeneously strained. The strain is produced by surrounding nanocrystals in the polycrystalline semiconductor film and carries information about the intercrystalline interactions. The measurements are done non destructively and without additional sample preparation or X-ray beam nanofocusing.

The demonstrated technique provides a way for connecting variations in the properties of individual crystallites inside of a working solar cell to the resulting energy conversion efficiency.

O 84.3 Fri 9:45 H2

Investigations of chemical gradients in $\mathrm{Cu(In,Ga)Se_2}$ thin film solar cells grown on polyimide substrate by high spatially resolved cathodoluminescence microscopy — •Stefan Ribbe[1,2], Andreas Rahm[1], Frank Bertram[2], and Jürgen Christen[2] — [1]Solarion AG, Ostende 5, 04288 Leipzig, Germany — [2]Institute for Experimental Physics, Otto-von-Guericke-Universität Magdeburg, Germany

Optical properties of $\mathrm{Cu(In,Ga)S_2}$(CIGS)-absorber layers for thin film solar cells have been studied by high spatially resolved cathodoluminescence (CL) at low temperature (T = 5K) to investigate lateral und vertical changes of the composition within the quaternary absorber. CIGS layers were grown on flexible polyimide foil by using an ion-beam assisted roll-to-roll process. To ensure high efficiency sodium fluoride was evaporated by an additional source during the process. The substrate temperature was varied above the standard value enabled by using an advanced polyimide substrate resisting higher temperatures. Cross sections of the thin film solar cells were prepared to investigate the vertical distribution of composition and its changes influenced by the substrate temperature. IV measurements showed an increase of the efficiency with higher substrate temperature suggesting less fluctuation of the composition and a smoother vertical gallium gradient. Furthermore a variation of the sodium content was made by variation of the evaporation temperature. Integral luminescence properties were investigated which showed a red shift and a broadening of the main peak with increased sodium content.

O 84.4 Fri 10:00 H2

Admittance spectroscopy on $\mathrm{Cu(In,Ga)Se_2}$ solar cells with respect to sodium content — •Felix Daume[1,2], Andreas Rahm[1], and Marius Grundmann[2] — [1]Solarion AG, Ostende 5, 04288 Leipzig, Germany — [2]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, 04103 Leipzig, Germany

Solar cells based on $\mathrm{Cu(In,Ga)Se_2}$ (CIGSe) absorbers deposited on flexible polyimide substrate enable cheap manufacturing with roll-to-roll equipment and the application in new environments such as low-load rooftops. Among present thin film flexible solar cell technologies, CIGSe achieves the highest efficiencies. The proper incorporation of sodium into the CIGSe absorber is indispensable to achieve these high efficiencies. In this study, sodium fluoride is co-evaporated during CIGSe deposition.

CIGSe solar cells with different sodium contents were investigated by admittance spectroscopy. We calculated activation energies for the N1 signature which, in literature, is widely attributed to defects. Overall concentrations and density profiles across the band gap were derived for this signature. Additionally, we derived the net doping of the CIGSe absorbers from capacitance-voltage measurements. A model based on defects at the CdS(n-type)/CIGSe(p-type) interface is proposed to explain our observations with respect to the sodium content.

O 84.5 Fri 10:15 H2

High-resolution Spectroscopic Mapping of Polymer Fullerene Blend Films for Organic Solar-Cell Applications — Xiao Wang, Kai Braun, Alfred J. Meixner, and •Dai Zhang — Institute of Physical and Theoretical Chemistry, Uni. Tübingen, Tübingen

Polymers and fullerenes are widely employed in the field of organic solar cells as the electronic donors and acceptors. The morphology and the photo-physical properties of the polymer and fullerenes blends at nanometer scale are critical for achieving a high performance of the solar cells. Employing a home-built parabolic mirror assisted apertureless near-field optical (Raman and photoluminescence) microscope, we demonstrated high resolution near-field spectroscopic mappings of the polymer:fullerene blend films. Our investigation focused on the additive effect for a C-PCPDTBT:PCBM blend film. From the simultaneously recorded morphology and spectroscopic information, the interplay among the blend film morphology, the local donor and acceptor molecular distributions, and the photoluminescence quenching efficiency were discussed. The PL and Raman signals of the electron donor and acceptor have been probed at an optical resolution of approximately 10 nm which allow the direct identification of the chemical nature of the different domains. Moreover, we were able to reveal and quantify the local quenching, which is related to the electron transfer from donor to acceptor.

O 84.6 Fri 10:30 H2

Investigation of the s-shape caused by the hole selective layer in organic bulk heterojunction solar cells — •Lothar Sims[1,2], Ulrich Hörmann[2], René Kogler[3], Roland Steim[4], Wolfgang Brütting[2], and Pavel Schilinsky[1] — [1]Belectric OPV GmbH, Landgrabenstr. 94, 90443 Nürnberg — [2]University of Augsburg, Institute of Physics, Universitätsstr. 1, 86135 Augsburg — [3]Evonik Industries AG, Kirschenallee, 64293 Darmstadt — [4]STORM Energy GmbH, Rathenauplatz 2, 90489 Nürnberg

During the operation period of an organic solar cell different failure mechanisms can occur which limit the lifetime of the device. Among these failure mechanisms the so called s-shape or second diode, where the current density-voltage (JV) curve bends towards the origin in the

4th quadrant, plays an important role. We investigated the origin of the s-shape caused by the hole selective layer (HSL) using N,N'-bis(3-methylphenyl)-N,N'-bis(phenyl)-benzidine (TPD) coevaporated with different amounts of Dipyrazino[2,3-f:2',3'-h]quinoxaline-2,3,6,7,10,11-hexacarbonitrile (HATCN) as a model system. The low glass transition temperature of TPD allows investigating the impact of WF and mobility of the HSL on device performance and thus s-shape independently of each other. The observed JV-curves were simulated by solving the drift-diffusion, i.e. continuity and Poisson equations numerical via the program PC1D. While WF rather influences the open circuit voltage, mobility seems to be the reason for the s-shape. The results show that an accumulation of holes near the hole selective/semiconductor layer interface might be responsible for the observed s-shape.

O 84.7 Fri 10:45 H2

The role of defects in nanocrystalline zinc oxide interlayers for polymer-based solar cells — •Sebastian Wilken, Dorothea Scheunemann, Florian Witt, Jürgen Parisi, and Holger Borchert — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky-Str. 9-11, 26129 Oldenburg, Germany

In polymer-based bulk heterojunction solar cells, the absorber blend has intrinsically no preferential transport direction for photogenerated charge carriers due to the statistical intermixing of both the donor and acceptor phase. Therefore, additional charge-selective interfacial layers, which are semipermeable membranes for either electrons or holes in an ideal case, are widely used in order to achieve efficient charge extraction at the respective contacts. One well established material for electron collection is zinc oxide (ZnO), which can be processed at moderate temperatures and deposited via solution-based techniques in form of colloidal nanocrystals (NCs). Here, we discuss the influence of defect states in interlayers made of ZnO NCs on the overall solar cell performance. For that purpose, ZnO NCs with different surface-to-volume ratios were wet-chemically synthesized and introduced into indium tin oxide-free polymer solar cells in the inverted device architecture. As indicated by photoluminescence, we show that surface defects play a more and more dominant role with decreasing NC size and, thus, limit the photovoltaic efficiency. For a more detailed analysis of the involved defect states, photo-induced current transient spectroscopy (PICTS) was performed for devices with varying amount of surface defects.

O 84.8 Fri 11:00 H2

Solar diode sensor — •Hao Shen[1], Martin Hoffmann[1], Juan Daniel Prades[2], Francisco Hernandez-Ramirez[3], and Andreas Waag[1] — [1]Institute of Semiconductor Technology, TU Braunschweig, D-38105 Braunschweig, Germany — [2]Department of Electronics, Uni. Barcelona, E-08028 Barcelona, Spain — [3]Catalonia Institute for Energy Research (IREC), E-08930 Barcelona, Spain

The nanodevice architecture presented here has been designed to overcome the current issues in gas sensor technologies: reducing power consumption and lowering operating temperature. Conductometric sensors based on semiconductor metal oxides need the continuous supply of the energy in the form of heat or UV light, to activate the chemical interaction between gases and the sensing surface. New concepts for energy harvesting units as an in-built module are demanded to make self-powered gas sensors. Herein we report a solar diode sensor (SDS) based on new designed CdS@n-ZnO/p-Si nanoelements which unifies gas sensing (CdS@n-ZnO) and solar energy harvesting (n-ZnO/p-Si diode) functionalities in a singular material unit and device. The SDS sensing mechanism (change of open circuit voltage), in comparison to the well-known conductometric sensors (change of resistance), is systematically studied and explained in terms of gas-material surface interactions and the subsequent changes in the doping level (ND), which is manifested in the variation of Voc in CdS@n-ZnO/p-Si. The fabricated SDS was capable of quantitatively detecting oxidising and reducing gases with reproducible response at room temperature and without the need of any other energy sources except solar illumination.

O 84.9 Fri 11:15 H2

Simulation of temperature distribution in ZnO:Al thin films for laser annealing experiments — •Christian Isenberg, Cay-Christian Kalmbach, Daniyal Sattarian, Uwe Stute, and Alexander Horn — Laser Zentrum Hannover e.V., Hollerithallee 8, 30419 Hannover, Germany

Transparent Conducting Oxides (TCOs) have become widespread as transparent electrodes in photovoltaics and transparent electronics. Thermal post deposition treatments by furnace annealing have shown to improve the electrical and optical properties of TCO thin films. Laser annealing of TCOs allows control over the peak temperature as well as the spatial and temporal temperature distributions of TCO thin films and substrates, preserving the substrate by heating only the TCO layer. Therefore, treating TCOs with tailored laser radiation allows larger temperature than furnace annealing even on temperature sensitive substrates. Numerical calculations using Crank-Nicolson method have been conducted to estimate the temperature distribution in ZnO:Al thin films during laser annealing process. In the special case of temperature-independent material parameters, the numerical solution is reduced to an analytical solution, determined by convolution of the heating source term with a Green's function for a geometry of a thin film on a semi-infinite substrate. Numerical results are compared to temperature measurements, done by a thermographic camera during laser annealing process.

Coffee break

O 84.10 Fri 11:45 H2

Selective laser ablation of Al_2O_3 passivation layers from optically black silicon surfaces — •Martin Otto[1], Katharina Widder[1], Tino Rublack[1], Matthias Zilk[2], Thomas Käsebier[2], Gerhard Seifert[1], and Ralf B. Wehrspohn[3] — [1]Martin-Luther-University Halle-Wittenberg, Institute of Physics -μ MD Group, Heinrich-Damerow-Strasse 4, 06120 Halle, Germany — [2]Friedrich Schiller University Jena, Institute of Applied Physics, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Fraunhofer Institute for Mechanics of Materials Halle, Walter-Hülse-Str. 1, 06120 Halle, Germany

Inductive coupled plasma reactive ion etching (ICP-RIE) of silicon enables excellent broad band and wide angle antireflective surface properties. The stochastically emerging needle like nano-structures let the silicon surface appear optically black due to its high absorption coefficient of over 97% integrated from 300 nm to 1175 nm. Concomitant, highly enhanced surface recombination is introduced. The latter, may be effectively suppressed by a well suited passivation layer of Al_2O_3 deposited by thermal ALD. Laser ablation is commonly used in the PV industry to open local contact areas in dielectric passivation stacks. In this work we show the feasibility to ablate alumina thin films from nano-structured black silicon (b-Si) solar cell front surfaces. Microstructural geometric analysis by focussed ion beam and SEM reveal certain structural changes in the zone of ablation which are believed to be beneficial for contact formation. Simultaneously, neither the deposition of Al_2O_3 layers of varying thickness nor their ablation lead to a very significant degradation of the optical surface properties.

O 84.11 Fri 12:00 H2

Surface Modification of Nano-Textured Black Silicon for Photovoltaic Applications — •Michael Algasinger[1], Svetoslav Koynov[1], Julie Paye[1], Florian Werner[2], Max Bernt[1], Martin S. Brandt[1], and Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany — [2]Institute for Solar Energy Research Hamelin, Am Ohrberg 1, 31860 Emmerthal, Germany

The morphology and the electronic properties of nano-textured silicon, obtained by a metal-catalyzed wet etching process and its improvement by an additional chemical treatment are examined with regard to solar cell applications. Photoluminescence and optical reflectivity measurements show evidence for a nano-porous silicon (np-Si) phase in the as-prepared nanostructure. It is found that an additional wet-chemical treatment removes the np-Si fraction and significantly alters the surface of the nanostructure. Cross-sectional scanning electron microscopy images reveal a drastic reduction of the surface area, to values of only 3 - 6 times of that of a planar surface. Electron spin resonance measurements were performed to investigate the type and quantity of defects induced by the nano-texturing process. First results on the passivation of surface defects via atomic layer deposition of Al_2O_3 are presented. Photoconductance decay measurements of passivated nanostructures, which received the additional post-etching treatment, show a significant increase in effective carrier lifetimes.

O 84.12 Fri 12:15 H2

Surface morphology of black silicon produced by metal-catalyzed wet etching — •Maximilian Bernt, Michael Algasinger, Svetoslav Koynov, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

Nano-textured silicon, also referred to as black silicon (b-Si), is a material with an optically graded surface, which shows reflectivity as low as 1 - 5 % in the whole range of Si absorption and additional light trapping effects. Due to its unique optical properties, b-Si is an interesting material for photovoltaic applications. However, b-Si produced by Au-catalyzed wet etching of crystalline Si (c-Si) wafers exhibits a nano-porous silicon (np-Si) phase in the as-prepared nano-structure. This np-Si phase leads to an increased surface area which could alter the electrical properties significantly. The formation of the nano-texture was investigated at different stages of the etch process by cross sectional scanning electron microscopy. The evolution of the np-Si phase with increasing etch time was observed by photoluminescence and optical reflectivity measurements. In addition, the influence of the doping level of n- and p-type c-Si substrates on the etch process and the morphology of the resulting nano-texture was studied.

O 84.13 Fri 12:30 H2

Valence band offsets estimation of Al_2O_3 films on silicon by XPS and UPS measurements — •Johannes Ziegler[1], Volker Naumann[2], Martin Otto[1], Alexander Sprafke[1], and Ralf B. Wehrspohn[1,3] — [1]Martin-Luther-University Halle-Wittenberg, Institute of Physics, Halle, Germany — [2]Fraunhofer Center for Silicon Photovoltaics CSP,Halle, Germany — [3]Fraunhofer Institute for Mechanics of Materials Halle, Halle, Germany

A quantitative measurement of valence band offsets in isolator-silicon junctions might help to realize heterojunction devices such like semiconductor-isolator-semiconductor (SIS) solar cells. We measured XPS and UPS spectra of thin (2–50 nm thick) Al_2O_3 films deposited on silicon by thermal ALD. The valence band offsets of these structures are estimated from the XPS spectra using the method of Kraut et.al. [1] . A slight trend in the valence band offsets 3.3–4.5 eV with increasing film thickness 2–50 nm was calculated from the XPS spectra. To estimate the valence band offsets from the UPS spectra 3.3–3.4 eV of 2–10 nm thick Al_2O_3 on silicon, a simple straight forward approach based on linear regression of the spectra on the band edges is used. We compare the results of both measurements and discuss possible sources for the measured increase of the valence band offset with increasing Al_2O_3 film thickness.

[1] A. Kraut, R. W. Grant, J. R. Waldrop and S. P. Kowalczyk, Phys. Rev. Lett. 44,p.1620 (1982), http://link.aps.org/doi/10.1103/PhysRevLett.44.1620

O 84.14 Fri 12:45 H2

Charge trapping in Al2O3 passivation layers for silicon solar cells — •Paul Jordan[1], Frank Benner[1], Ingo Dirnstorfer[1], and Thomas Mikolajick[1,2] — [1]NaMLab gGmbH, Dresden, Germany — [2]Lehrstuhl für Nanoelektronische Materialien, TU Dresden, Dresden, Germany

Novel highly efficient silicon solar cells require an excellent level of surface passivation, to minimize recombination losses of photo-generated carriers. During the last decade, the dielectric Al2O3 became the material of choice for the passivation of p-type silicon. The excellent passivation properties are mainly caused by negative charges located within the dielectric. In this study the origin of the negative charges is investigated using capacitance-voltage and microwave detected photoconductivity measurements. It will be shown that the negative charges are partly caused by electrons, injected from silicon into the dielectric. The trapping dynamics are analyzed by the means of the post program discharge technique, which is commonly applied for memory devices. Furthermore, the trapping and detrapping rates depend on the thickness of the ultra-thin SiO2 interface between Si and Al2O3. For an interface thickness of about 2 nm, the asymmetry of trapping and detrapping rates significantly enhances the negative charge density. As a consequence an optimum interface thickness is essential for the excellent passivation property of Al2O3.

O 84.15 Fri 13:00 H2

Investigation of carrier traps in pn-junctions of fully-processed silicon photovoltaic cells — •Teimuraz Mchedlidze, Leopold Scheffler, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

Mesa-diodes with a surface area about 1 mm^2 and a height of 50 μm were fabricated on top of fully-processed Si photovoltaic-cell wafers for detection and investigation of carrier traps in pn-junctions. All fabrication steps were performed at room temperature and fully preserved the initial structure of the cell inside the mesa-diode. Schottky diodes were fabricated on neighbor locations of the wafers after etching off the PV-cell structure to a depth of 50 μm. The DLTS spectra detected for the mesa- and Schottky-diodes show significant difference, namely the deep carrier traps detected in the mesa-structures were below the detection limit in the Schottky-diodes. Profiling of the trap density for the mesa-diodes showed a steep decrease with increasing distance from the pn-junction. Parameters of the detected traps, their possible origin and reasons for the differences between spectra detected for mesa- and Schottky-diodes are presented and discussed.

O 84.16 Fri 13:15 H2

Iron acceptor association in compensated multicrystalline silicon — •Christian Möller[1,2], Kevin Lauer[1], Fabien Gibaja[3], Til Bartel[3], and Fritz Kirscht[3] — [1]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, SolarZentrum Erfurt, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany — [2]TU Ilmenau, Institut für Physik, Weimarer Str. 32, 98693 Ilmenau, Germany — [3]Calisolar GmbH, Magnusstraße 11, 12489 Berlin

Monitoring the acceptor concentration in compensated multicrystalline silicon by a minority-charge carrier lifetime measurement is applicable for production control due to the fast and easy lifetime measurement. The iron acceptor pair association is studied for several acceptors position dependent over the whole height of a compensated multicrystalline ingot. Acceptor pair and height dependent induced differences in the defect kinetics are visible. The calculated position depending doping concentrations of several ingots from charge carrier lifetime measurements are discussed and compared with the expected doping concentration calculated via Scheil equation.

O 84.17 Fri 13:30 H2

Femtosecond laser processed sulfur-emitter solar cells — •Thomas Gimpel[1], Kay-Michael Günther[2], Anna Lena Baumann[1], Wolfgang Schade[1], and Stefan Kontermann[1] — [1]Fraunhofer Heinrich Hertz Insitute, EnergieCampus, Am Stollen 19B, 38640 Goslar, Germany — [2]Energieforschungszentrum Niedersachsen, EnergieCampus, Am Stollen 19B, 38640 Goslar, Germany

A simple fs-laser process enables structuring and sulfur incorporation simultaneously. This process is applied on a single side to different silicon substrates independent from the crystal structure. Without any advanced solar engineer processes like passivation, dopant source layer deposition, its diffusion and removal, efficiencies of 8.2% are achieved, at present. Due to an incorporated intermediate band this material has the potential to convert infrared light even at wavelengths below the silicon band gap. New applications e.g. in a crystalline silicon tandem solar cell are under development.

O 85: Transport: Topological Insulators (jointly with DS, HL, MA, and TT)

Time: Friday 9:30–13:00 Location: H18

O 85.1 Fri 9:30 H18

Structure factor of a weakly interacting helical liquid — •Suhas Gangadharaiah[1,2], Thomas L. Schmidt[2], and Daniel Loss[2] — [1]Indian Institute of Science Education and Research, Bhopal, India — [2]Department of Physics, University of Basel, CH-4056 Basel, Switzerland

We calculate the density structure factor $S(q,\omega)$ of a weakly interacting helical liquid in the presence of a magnetic field B. The latter opens a gap of width $2B$ in the single-particle spectrum $\epsilon_\pm(k)$, and leads to a strongly nonlinear spectrum near $k = 0$. For chemical potentials $\mu > B$, the system then behaves as a nonlinear helical Luttinger liquid, and a mobile-impurity analysis reveals interaction-dependent power-law singularities in $S(q,\omega)$. For $\mu < B$, the low-energy excitations are gapped, and we determine $S(q,\omega)$ by using an analogy to exciton physics. We discuss the implications of the magnetic field induced non-linear spectrum on the Coulomb drag between the helical liquids.

O 85.2 Fri 9:45 H18

Strongly interacting Majorana modes in an array of Josephson junctions — Fabian Hassler[1] and •Dirk Schuricht[2] — [1]Institute for Quantum Information, RWTH Aachen University — [2]Institute for Theory of Statistical Physics, RWTH Aachen University

An array of superconducting islands with semiconducting nanowires in the right regime provides a macroscopic implementation of Kitaev's toy model for Majorana wires. We show that a capacitive coupling between adjacent islands leads to an effective interaction between the Majorana modes. We demonstrate that even though strong repulsive interaction eventually drive the system into a Mott insulating state the competition between the (trivial) band-insulator and the (trivial) Mott insulator leads to an interjacent topological insulating state for arbitrary strong interactions.

O 85.3 Fri 10:00 H18

All-electrical measurement of crossed Andreev reflection in topological insulators — •Rolf W. Reinthaler[1], Patrik Recher[2], and Ewelina M. Hankiewicz[1] — [1]Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Institute for Mathematical Physics, Technical University Braunschweig, Braunschweig, Germany

Using a generalized wave matching method we solve the full scattering problem for quantum spin Hall insulator (QSHI) - superconductor (SC) - QSHI junctions. We find that for systems narrow enough so that the bulk states in the SC part couple both edges, the crossed Andreev reflection (CAR) is significant and the electron cotunneling (T) and CAR become spatially separated. We study the effectiveness of this separation as a function of the system geometry and the level of doping in the SC. Moreover, we show that the spatial separation of both effects allows for an all-electrical measurement of CAR and T separately in a 5-terminal setup or by using the spin selection of the quantum spin Hall effect in an H-bar structure [1].

We acknowledge financial support by the DFG grant HA 5893/3-1.

[1] R. W. Reinthaler, P. Recher, and E. M. Hankiewicz, arXiv:1209.5700 (2012)

O 85.4 Fri 10:15 H18

Zero-voltage conductance peak from weak antilocalization in a Majorana nanowire — •Michael Wimmer[1], Dimitri Pikulin[1], Jan Dahlhaus[1], Henning Schomerus[2], and Carlo Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, The Netherlands — [2]Department of Physics, Lancaster University, United Kingdom

We show that weak antilocalization by disorder competes with resonant Andreev reflection from a Majorana zero-mode to produce a zero-voltage conductance peak of order e^2/h in a superconducting nanowire. The phase conjugation needed for quantum interference to survive a disorder average is provided by particle-hole symmetry - in the absence of time-reversal symmetry and without requiring a topologically nontrivial phase. We identify methods to distinguish the Majorana resonance from the weak antilocalization effect.

O 85.5 Fri 10:30 H18

Spectral properties of disordered multi-channel Majorana wires — •Patrick Neven, Dmitry Bagrets, and Alexander Altland — Institut für Theoretische Physik, Universität zu Köln, Köln, Germany

Proximity coupled multi-channel spin-orbit quantum wires may support midgap Majorana states at the ends. We study the fate of these Majorana fermions in the presence of disorder in such wires. Inspired by the widely established theoretical methods of mesoscopic superconductivity, we develop a quasiclassical approach which is valid in the limit of strong spin-orbit coupling. A numerical solution of the Eilenberger equation reveals that disordered topological wires are prone to the formation of a zero-energy anomaly (class D impurity spectral peak) in the local density of states which shares the key features of a Majorana peak. We also find that the $\mathbb{Z}_2$ topological invariant distinguishing between the state with and without Majorana fermions (symmetry class B and D, resp.) is related to the Pfaffians of quasiclassical Green's functions.

O 85.6 Fri 10:45 H18

Topological invariants and interacting one-dimensional fermionic systems — •Salvatore R. Manmana[1,2,3], Andrew M. Essin[3], Reinhard M. Noack[4], and Victor Gurarie[3] — [1]Institut für Theoretische Physik, Universität Göttingen, Germany — [2]JILA, University of Colorado and NIST, Boulder (CO), USA — [3]Department of Physics, University of Colorado at Boulder, USA — [4]Fachbereich Physik, Philipps-Universität Marburg, Germany

We study one-dimensional, interacting, gapped fermionic systems described by variants of the Peierls-Hubbard model, and we characterize their phases via a topological invariant constructed out of their Green's functions. We demonstrate that the existence of topologically protected, zero-energy states at the boundaries of these systems can be tied to the value of the topological invariant, just like when working with the conventional, non-interacting topological insulators. We use a combination of analytical methods and the numerical density matrix renormalization group method to calculate the values of the topological invariant throughout the phase diagrams of these systems, thus deducing when topologically protected boundary states are present. We are also able to study topological states in spin systems because, deep in the Mott insulating regime, these fermionic systems reduce to spin chains. In this way, we associate the zero-energy states at the end of an antiferromagnetic spin-1 Heisenberg chain with a topological invariant equal to 2.

O 85.7 Fri 11:00 H18

Fluctuation driven topological Hund insulator — •Jan Carl Budich[1], Bjoern Trauzettel[2], and Giorgio Sangiovanni[2] — [1]Department of Physics, Stockholm University, Se-106 91 Stockholm, Sweden — [2]Institute for theoretical physics and astrophysics, 97074 Würzburg, Germany

We investigate in the framework of dynamical mean field theory a two-band Hubbard model based on the Bernevig-Hughes-Zhang Hamiltonian describing the quantum spin Hall (QSH) effect in HgTe quantum wells. In the presence of interaction, we find that a system with topologically trivial non-interacting parameters can be driven into a QSH phase at finite interaction strength by virtue of local dynamical fluctuations. For very strong interaction, the system reenters a trivial insulating phase by going through a Mott transition. We obtain the phase diagram of our model by direct calculation of the bulk topological invariant of the interacting system in terms of its single particle Green's function.

15 min. break

O 85.8 Fri 11:30 H18

Floquet Topological Quantum Phase Transitions in the Wen-Plaquette Model — •Victor Manuel Bastidas Valencia, Clive Emary, Gernot Schaller, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Our aim in this talk is to describe the nonequilibrium behavior of the topological quantum phase transition in the Ac-driven Wen-plaquette model. We show that under the effect of a nonadiabatic driving the system exhibits a novel topological phase. We define generalized topological order parameters by considering cycle-averaged expectation values of string operators in a Floquet state.

O 85.9 Fri 11:45 H18

Fermion-parity anomaly of the critical supercurrent in the quantum spin-Hall effect — •Jan Dahlhaus[1], Dmitry Pikulin[1], Timo Hyart[1], Henning Schomerus[2], and Carlo Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, Niederlande — [2]Department of Physics, Lancaster University, United Kingdom

The helical edge state of a quantum spin-Hall insulator can carry a supercurrent in equilibrium between two superconducting electrodes (separation L, coherence length ξ). We calculate the maximum (critical) current I_c that can flow without dissipation along a single edge, going beyond the short-junction restriction $L \ll \xi$ of earlier work, and find a dependence on the fermion parity of the ground state when L becomes larger than ξ. Fermion-parity conservation doubles the critical current in the low-temperature, long-junction limit, while for a short junction I_c is the same with or without parity constraints. This provides a phase-insensitive, dc signature of the 4π-periodic Josephson effect.

O 85.10 Fri 12:00 H18

Topological kicked rotators — •Jan Dahlhaus[1], Jonathan Edge[1], Jakub Tworzydlo[2], and Carlo Beenakker[1] — [1]Instituut-

Lorentz, Universiteit Leiden, Niederlande — [2]Institute of Theoretical Physics, University of Warsaw, Poland

Topology is a nice mathematical concept that can have profound consequences on condensed matter systems. Maybe the most prominent examples are the quantum Hall effect, the quantum spin Hall effect and the 3D topological insulator. I will present a way to realize the ideas of band topology in a well-known and intensively-studied model - the quantum kicked rotator. This allows to study the Anderson localization properties of topological phase transitions numerically in a very efficient way, especially in higher dimensions. Furthermore it may open a way for experimental measurements of this transition behaviour with cold atomic gases in optical lattices.

O 85.11 Fri 12:15 H18

Theory of correlated topological insulators with broken axial spin symmetry — •Stephan Rachel — TU Dresden, 01069 Dresden, Germany

The two-dimensional Hubbard model defined for topological band structures exhibiting a quantum spin Hall effect poses fundamental challenges in terms of phenomenological characterization and microscopic classification. We consider weak, moderate, and strong interactions and argue that the resulting phase diagrams depend on the microscopic details of the spin orbit interactions which give rise to the non-trivial topology. In particular, it turns out that there is a crucial difference between models with broken and with conserved axial spin symmetry. These results suggest that there is a general framework for correlated 2D topological insulators with broken axial spin symmetry.

[1] Rachel, LeHur, PRB 82, 075106 (2010)
[2] Schmidt, Rachel, von Oppen, Glazman, PRL 108, 156402 (2012)
[3] Cocks, Orth, Rachel *et al.*, PRL 108, 205303 (2012)
[4] Reuther, Thomale, Rachel, PRB 86, 155127 (2012)

O 85.12 Fri 12:30 H18

Interaction effects on almost flat surface bands in topological insulators — •Matthias Sitte, Lars Fritz, and Achim Rosch — Universität zu Köln, Institut für Theoretische Physik, Zülpicher Str. 77, 50937 Köln, Deutschland

We investigate ferromagnetic instabilities of the two-dimensional helical Dirac fermions hosted on the surface of three-dimensional topological insulators. We concentrate on ways to increase the role of interactions by means of modifying the bulk properties which in turn changes the surface Dirac theory characteristics. We discuss both long-ranged Coulomb interactions controlled by the dimensionless coupling constant $\alpha = e^2/(\hbar \epsilon v_F^{\mathrm{surf}})$ as well as short-ranged Hubbard-like interactions of strength U which can induce spontaneous surface ferromagnetism, thereby gapping the surface Dirac metal. In both cases, we find that a prerequisite for observing this effect is to reduce the Fermi velocity v_F^{surf}, and we consider different mechanisms to achieve this. While for long-ranged Coulomb interactions we find that screening hinders ferromagnetism, for short-ranged interactions screening is not that vital and the instability can prevail.

O 85.13 Fri 12:45 H18

Local spin susceptibility and surface states in doped three-dimensional topological insulators with odd-parity superconducting pairing symmetry — •Björn Zocher[1,2] and Bernd Rosenow[1] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04103 Leipzig, Germany — [2]Max Planck Institut für Mathematik in den Naturwissenschaften, D-04103 Leipzig, Germany

We investigate characteristic features in the spin response of doped three-dimensional topological insulators with odd-parity unequal-spin superconducting pairing. To get insight into the nature of the superconducting pairing symmetry, we show that the odd-parity unequal-spin pairing can be mapped onto p-wave pairing and that these systems have gapless Majorana surface modes. The Majorana modes contribute to the local spin susceptibility, giving rise to a characteristic temperature behavior of the Knight shift and the spin-lattice relaxation time in magnetic resonance experiments. Because of their different decay lengths, the Majorana modes can be observed and clearly distinguished from the Dirac modes of the topological insulator by local probes which allow for a depth-controlled study of the electron spins on the nanometer length scale.

O 86: Plasmonics and Nanooptics VI

Time: Friday 10:30–13:00 Location: H36

O 86.1 Fri 10:30 H36

Modelling attosecond dynamics: tracking collective excitations — •Andrey Moskalenko, Yaroslav Pavlyukh, Jonas Wätzel, and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

The emergence of attosecond light sources is undoubtedly one of most exciting developments in science in the last decade and is expected to change significantly the face of physics, chemistry and biology research. A series of benchmark experiments on the attosecond electron dynamics in atomic, molecular and condensed matter systems reveal fundamentally new processes taking place in this time regime and evidence the high potential of this rapidly growing field. One of the fundamental open questions, which can be targeted with these new experimental tools, is how an inherent collective response of matter is formed on an ultrashort, possibly attosecond time scale. In this presentation we report on our progress towards modelling attosecond electron dynamics in clusters. Combining quantum chemical computation [1] with quantum kinetic methods we calculate the time-dependent light absorption and refraction in fullerene that serve as indicators for the emergence of collective modes. We trace on an attosecond time scale the collective excitations in this finite system and find distinct new features in this regime [2]. Finally, we discuss how to observe the predicted dynamics in a XUV-pump XUV-probe or in an attosecond streaking experiments.

[1] Y. Pavlyukh and J. Berakdar, Chem. Phys. Lett. 468, 313 (2009).
[2] A.S. Moskalenko, Y. Pavlyukh, and J. Berakdar, Phys. Rev. A 86, 013202 (2012).

O 86.2 Fri 10:45 H36

Plasmon-induced fluorescence and electroluminescence from porphine molecules on GaAs(110) in a scanning tunneling microscope — •Svenja Mühlenberend, Natalia L. Schneider, Markus Gruyters, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

An STM tip can be used to excite luminescence from atomic scale structures. For the investigation of molecular fluorescence, however, the coupling to metallic substrates has been a major issue as it largely inhibits fluorescence. The decoupling of molecules by e.g. multilayer arrangements or salt layers has been used to circumvent this difficulty. Here, we report on fluorescence from tetraphenyl-porphine molecules on a semiconductor (GaAs(110)) for very low coverages of less than 5% of a monolayer without any decoupling layer. Evidence for intramolecular Q-band transitions is found in the fluorescence spectra. The processes involved in exciting this molecular fluorescence will be discussed.

O 86.3 Fri 11:00 H36

Single giant pseudoconjugated macrocycles mimic light-harvesting complexes — Vikas Aggarwal[1], Alex Thiessen[2], Alisa Idelson[1], •Dominik Würsch[3], Thomas Stangl[3], Florian Steiner[3], Stefan-S. Jester[1], Jan Vogelsang[3], Sigurd Höger[1], and John Lupton[3] — [1]University of Bonn, Bonn, Germany — [2]University of Utah, Salt Lake City, Utah, USA — [3]University of Regensburg, Regensburg, Germany

Natural light-harvesting complexes have long served as model systems of the physics of molecular excitons. Synthetic model systems which mimic specific aspects of exciton coupling would allow investigating the effects of coupling in a highly defined system. Here we introduce giant shape persistent macrocycles of carbazole-enthynylene units of 7 nm diameter. Fully conjugated macrocycles are generally considered to be non-emissive because the fundamental oscillator mode is dipole forbidden. For every electron which moves in one direction there is another moving in exactly the opposite direction, resulting in a vanishing dipole moment. Spontaneous fluctuations in the conjugation lead to strongly allowed fluorescence of the system which enables single molecule studies of the emitter. We find that the conjugation varies with time resulting in jumps in the linear dichroism. The conjugation of the macrocycle is dynamically interrupted leading to more than one chromophore being present. Surprisingly, we find that the emission polarization can rotate without a change in transition energy, implying that the different chromophores on the ring remain susceptible to the same dielectric environment.

O 86.4 Fri 11:15 H36

Scanning probe techniques in quantum plasmonics — •Andreas W. Schell, Philip Engel, Günter Kewes, and Oliver Benson — Humboldt-Universität zu Berlin, AG Nanooptik

In recent years, scanning probe technologies like atomic force microscopy have developed into a versatile tool for nano-manipulation and nano-assembly tasks [1]. Using nano-manipulation approaches it has become possible to realize different configurations of the same constituents. Here, we will show the controlled coupling of a single photon emitting nitrogen vacancy (NV) center in nanodiamond to different plasmonic structures as well as its use as a probe for the local density of optical states (LDOS) at the nanoscale [2]. With the NV center glued to the tip of an atomic force microscope the LDOS is mapped out in a very controlled way in all three dimensions, giving insight into the local behavior of the emitter-plasmon coupling.

[1] A.W. Schell et al., Rev. Sci. Instrum. 82, 073709 (2011).
[2] A.W. Schell et al., Opt. Express. 19, 7914 (2011).

O 86.5 Fri 11:30 H36

Validity of the effective medium theory for hyperbolic layered materials in the presence of surface modes. — •Maria Tschikin[1], Philippe Ben-Abdallah[2], and Svend-Age Biehs[1] — [1]Carl von Ossietzky Universität, Institute of Physics, 26111 Oldenburg, Germany — [2]Laboratoire Charles Fabry, Institut d'Optique, CNRS, Université Paris- Sud, France

It is well known that the physics of periodic structures can be described by the effective medium theory (EMT) if the period of the structure is smaller than the wavelength of radiation. One example where the EMT is applied are bilayer structures with effective permittivity perpendicular $\epsilon_\perp$ and parallel $\epsilon_{||}$ to the optical axes. If both effective permittivities have different signs, i.e., $\epsilon_\perp\epsilon_{||} < 0$, than the dispersion relation for propagating modes inside the medium is hyperbolic. In these regions the local density of states can have large values in a broad frequency band which can be used for near-field energy conversion or broadband enhanced spontaneaus emission. We consider the particular case where surface modes appear inside the hyperbolic bands and show that the EMT can lead to wrong interpretations. In particular effects which are due to surface modes could be associated to hyperbolic modes. To this end, we compare exact S-matrix calculations with the results of EMT and determine the regions where EMT can lead not only to quantitatively but also to qualitatively wrong results.

O 86.6 Fri 11:45 H36

Nanoscale heat transfer: hyperbolic modes versus surface modes — •Svend-Age Biehs[1], Maria Tschikin[1], and Philippe Ben-Abdallah[2] — [1]Carl von Ossietzky Universität, Institute for Physics, 26111 Oldenburg, Germany — [2]Laboratoire Charles Fabry, Institut d'Optique, CNRS, Université Paris- Sud, France

The radiative heat flux at the nanoscale can be by orders of magnitude larger than that between two black bodies. Therefore, this effect is sometimes called super-Planckian thermal radiation. When considering polar materials like SiC, it was shown that at the nanoscale the dominant heat flux channel is due to surface phonon polaritons. Here, we show that for hyperbolic/indefinite materials one can also achieve very large heat fluxes without any surface modes. In this case, the dominant heat flux channel is due to frustrated total internal reflection modes. We show that this is a broad-band effect whereas the heat flux due to surface modes is a quasi-monochromatic effect which is preferable for applications in near-field thermophotovoltaics, for instance. Finally, we present exact calculations for multilayer structures and discuss the impact of hyperbolic modes and surface modes.

O 86.7 Fri 12:00 H36

Probing optical near-fields by photoemission of electrons with 1 nm resolution — •Sebastian Thomas[1], Michael Krüger[1], Michael Förster[1], Markus Schenk[1], and Peter Hommelhoff[1,2] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Gemany — [2]Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen, Germany

We present a new method of measuring optical near-field enhancement. In our experiments, we use a metal nanotip under laser illumination as an ultrafast source of photoelectrons. Some of the emitted electrons return to the tip surface within one optical cycle of the driving field, where they may gain energy by elastic rescattering [1]. This process crucially depends on the electric field strength in the immediate vicinity of the surface. By measuring the kinetic energy of rescattered electrons, we obtain the enhanced electric field strength within 1 nm from the tip surface [2]. This is close to the length scale of quantum plasmonics, and about an order of magnitude better than the previous record resolution [3].

Our results for the field enhancement factor at tungsten and gold tips are in good agreement with Maxwell simulations. Further simulations of nanotips with varying dielectric function give insight into the plasmonic characteristics of nanotips, which differ significantly from those of nanospheres.

[1] Krüger, Schenk, Hommelhoff, Nature 475, 78 (2011)
[2] Thomas et al., arxiv:1209.5195 (2012)
[3] Raschke et al., ChemPhysChem 6, 2197 (2005)

O 86.8 Fri 12:15 H36

Effect of size and shape of randomly distributed ZnO nanoneedle arrays on the localization of light fields — •Martin Silies[1], Manfred Mascheck[1], Slawa Schmidt[1], Janos Sartor[2], David Leipold[3], Takashi Yatsui[4], Kokoro Kitamura[4], Motoicho Ohtsu[4], Heinz Kalt[2], Erich Runge[3], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Karlsruhe Institute of Technology, Germany — [3]Technische Universität Ilmenau, Germany — [4]University of Tokyo, Japan

We report on measurements about the influence of size, shape and diameter of arbitrarily arranged ZnO nanostructures on the localization of light. We use coherent, ultra-broadband Second Harmonic (SH) microscopy to investigate the spatial localization of light in nm-sized ZnO needle arrays. Strong fluctuations of the SH intensity inside different ZnO needle geometries are observed [1].

Comparison of the SH intensity distributions with predictions based on one-parameter scaling theory indicate that SH fluctuations may be taken as a quantitative measure to classify the degree of localization [2]. Surprisingly, the strongest localization signatures are found for densely packed arrays of thin needles with diameters in the 30 nm range. Our results indicate that for sufficient high filling factors and small needle diameters near-field coupling between neighbouring needles governs the localization. These findings are supported by 3D-FDTD simulations using a Maxwell equation solver.

[1] Mascheck et al., Nat. Phot. 6, 293 (2012)
[2] Abrahams et al., Phys. Rev. Lett. 42, 673 (1979)

O 86.9 Fri 12:30 H36

Time-resolved near field microscopy of a metal particles breathing oscillation — •Matthias Brandstetter[1,2], Ralf Vogelgesang[3], and Markus Lippitz[1,2] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]University Stuttgart, Germany — [3]Carl von Ossietzky University Oldenburg, Deutschland

The localized surface plasmon resonance (LSPR) of a metal nanoparticle depends directly on the geometry and the dielectric constant of the nanoobject. Impulsive heating through a laser pulse launches acoustical oscillations of the whole particle. The mechanical oscillations lead to a local variation in the dielectric properties. Using an apertureless SNOM in a pump-probe configuration, we locally probe these changes of the dielectric properties of a nanoparticle on the picosecond timescale. The spatial resolution is defined by the near-field microscope (about 10 nm). The temporal resolution is just limited by the duration of the laser pulse, in our case to about one picosecond. This new device will allow us to investigate ultrafast processes on the nanoscale. We present our combination of an apertureless scanning near-field microscope and a pump probe setup as well as experimental results.

O 86.10 Fri 12:45 H36

Recent Progress in the Simulation of Plasmonic Systems with the DGTD Method — •Jens Niegemann — Institut für Feldtheorie und Höchstfrequenztechnik (IFH), ETH Zürich, Switzerland

Due to its flexibility and efficiency, the discontinuous Galerkin time-domain (DGTD) method has established itself as a popular method in the field of wave propagation. Here, we discuss our recent advances in using the DGTD method for the simulation of plasmonic and nanophotonic devices. In particular, we demonstrate how a memory-efficient formulation of curvilinear elements together with an implementation on graphics processing units (GPUs) significantly reduces the computational time. This allows large parameter scans or numerical optimizations with relatively little computational power.

O 87: Focussed Session: Solid-liquid Interfaces III

Time: Friday 10:30–13:00 Location: H31

O 87.1 Fri 10:30 H31

Nonintrusive Optical Visualization of Surface Nanobubbles — •Stefan Karpitschka[1], Erik Dietrich[2,3], James Seddon[2], Harold Zandvliet[3], Detlef Lohse[2], and Hans Riegler[1] — [1]MPI für Kolloid- und Grenzflächenforschung, Potsdam, Germany — [2]Physics of Fluids, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands — [3]Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Individual surface nanobubbles are visualized with nonintrusive optical interference-enhanced reflection microscopy [1], demonstrating that their formation is not a consequence of the hitherto used intrusive atomic force microscopy technique. We then use this new and fast technique to demonstrate that surface nanobubbles form in less than a few seconds after ethanol-water exchange, which is the standard procedure for their preparation, and examine how they react to temperature variations [2,3].

[1] R. Köhler, P. Lazar, and H. Riegler, Appl. Phys. Lett. 89, 241906 (2006).

[2] S. Karpitschka, E. Dietrich, J.R.T. Seddon, H.J.W. Zandvliet, D. Lohse, and H. Riegler, PRL 109, 066102 (2012).

[3] Nature Nanotechnology (Research Highlights) 7, 549 (2012).

O 87.2 Fri 10:45 H31

Studying confined liquids by using the thermal fluctuations of cantilevers — •Fei Liu, Sissi de Beer, Dirk van de Ende, and Frieder Mugele — MESA+, University if Twente

By analyzing the thermal fluctuations of atomic force microscopy (AFM) cantilevers, we characterize the distance-dependent interaction stiffness and dissipation in bulk/confined octamethylcyclotetrasiloxane (OMCTS), which exhibits short-range ordering (and hence forces) on confinement. In the measurement, the thermal fluctuations of the tip are recorded and parsed into segments as the tip approaches the surface. Each section is transformed to a power spectrum, which we fit to a simple harmonic model. From the fitted resonance frequency and quality factor, we extract the interaction stiffness and damping coefficient. The technique is validated by measuring the bulk viscosity with a blunt tip. Then the experiment is done with sharp tips. It is observed that the interaction stiffness matches well with theory prediction- exponentially decaying oscillatory cosine function w.r.t tip-surface distance. The damping displays non-monotonic behavior and thus deviates from continuum hydrodynamics.

O 87.3 Fri 11:00 H31

Structure and Dynamics of Ionic Liquid-Electrode Interfaces — •Peter Reichert[1], Jannis Ochsmann[1], Kasper Skov Kjaer[2], Tim Brandt van Driel[2], Martin Meedom Nielsen[2], Harald Reichert[3], Diego Pontoni[3], and Markus Mezger[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz — [2]Technical University of Denmark and Riso National Lab, Roskilde — [3]European Synchrotron Radiation Facility, Grenoble

Ionic liquids (ILs) are promising electrolytes for electrochemical double-layer capacitors with high energy storage densities. To understand and optimize their capacitance as well as charging and discharging processes, detailed information of the IL molecular scale structure and dynamics at interfaces, i.e. the spatial density profiles of the ions near an electrode, is highly desirable. Analysis of our in-situ high-energy x-ray reflectivity (XRR) experiments on IL-electrode interfaces under potential control revealed oscillatory profiles comprised of alternating anion and cation enriched regions. The relaxation dynamics of the interfacial structure upon potential variation was studied by time resolved XRR experiments on a sub-millisecond timescale. The molecular scale structure and its dynamics are set in relation to differential capacitance curves measured by impedance spectroscopy.

O 87.4 Fri 11:15 H31

Surface patterning by molecular polygons and stars: Designed 2D nanoarchitectures at the solid/liquid interface imaged by STM — •Stefan-S. Jester, Eva Sigmund, Nina Schönfelder, Lisa M. Röck, and Sigurd Höger — Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

The self-assembly of shape-persistent organic molecules at the solution/solid interface is an efficient bottom-up approach towards predictable 2D architectures. Scanning tunneling microscopy yields a submolecularly resolved insight into the monolayer structures. How do the nanoscale patterns - here: supported on graphite - depend on the shapes, sizes, and substituents of the adlayer building blocks? We recently focused on *molecular polygons* (triangles, squares, pentagons, and hexagons) with dithiophene corners and phenylene-alkynylene sides, as well as on *molecular stars*, polycyclic heteroaromatic hydrocarbons for which frustrated self-assembly leads to hierarchically organized superstructures with unit cells of up to 20 molecules. In my talk I will give insight into the relation between discrete geometry and supramolecular adlayers, show cocrystals of triangles and hexagons, and explain how large periodicities beyond 10 nm become accessible.

[1] S.-S. Jester, N. Shabelina, S. M. Le Blanc, S. Höger, *Angew. Chem. Int. Ed.* **2010**, *49*, 6101. [2] S.-S. Jester, E. Sigmund, S. Höger, *J. Am. Chem. Soc.* **2011**, *133*, 11062. [3] S.-S. Jester, E. Sigmund, L. M. Röck, S. Höger, *Angew. Chem. Int. Ed.* **2012**, *51*, 8555.

O 87.5 Fri 11:30 H31

Self-assembly of block copolymers at the air/water interface. — •Iryna Perepichka, Kateryna Borozenko, Antonella Badia, and Geraldine Bazuin — Department of Chemistry, University of Montreal, Montreal (QC), Canada

By investigation of a wide range of poly(styrene)-poly(4-vinyl pyridine) (PS-PVP) diblock copolymers and their supramolecular complexes with 3-n-pentadecylphenol (PDP), we have established the molecular parameters and experimental conditions that control the self-assembly of planar, strand and dot morphologies at the air/water interface. This has led to an extensive discussion concerning the mechanisms of nanopattern formation, including kinetic, molecular association, and dewetting contributions. We have shown that the use of high-boiling solvents (not usually used for Langmuir-Blodgett film preparation) can improve the nanostrand order.[1] In addition, we have provided a new interpretation of the phase transition plateau on surface pressure area isotherms of block copolymer Langmuir films with dot morphologies.[2] The ability to produce well-controlled nanopatterned films on various substrates has been demonstrated, and film stability has been verified. Removal of small molecules from the nanostructures has revealed the appearance of new substructure. Our studies form the basis for the use of ultrathin films as templates for nanolithography.

References: [1] Perepichka I.I., Badia, A., Bazuin, C.G. ACS Nano 2010, 4, 6825. [2] Perepichka I.I., Borozenko E., Badia, A., Bazuin, C.G. J. Am. Chem. Soc. 2011, 133, 19702.

O 87.6 Fri 11:45 H31

Molecular dynamics simulation of interfaces of gold nanorods — •Santosh Meena and Marialore Sulpizi — Condensed Matter Theory, Institute of Physics, Johannes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany

Nanorods are widely used in many areas such as drug delivery, photothermal cancer therapy, biochemical sensing and medical imaging. Growth of nanorods starts from small reasonably uniform gold seeds in a widely employed experimental technique, seed-mediated growth. In this technique ascorbic acid (a mild reducing agent), is added to aqueous cetyltrimethylammonium bromide (CTAB) solution of HAuCL4 for selective reduction of Au(III) to Au(I), followed by the addition of the seed solution which catalyze the reduction of Au(I) on their surface. Isotropic morphology breaking of the seeds results into anisotropic growth and thus formation of nanorods. However, the microscopic mechanism of symmetry breaking and anisotropic growth is still unknown. Therefore, we studied the adsorption mechanism of CTAB surfactant on different facets of gold, namely 110, 100 and 111 using molecular dynamics (MD) simulation. Atomistic models for different gold surfaces with CTAB surfactant in water were built using GROMOS 53A6 force-field parameters. Properties like, number densities of species and electrostatic potential were calculated across the gold-CTAB and CTAB-water interfaces in order to understand the adsorption of CTAB on the different gold surfaces. Higher density of adsorbed species were found on 110 and 100 facets than 111, this possibly results growth of the nanorod more in the direction of 111 facet.

O 87.7 Fri 12:00 H31

Calcium oxalate/water interfaces using ab initio Molecular Dynamics — •Leila Salimi Parvaneh[1,2], Davide Donadio[1], and Marialore Sulpizi[2] — [1]MPI for Polymer Research, Mainz — [2]Physics Department, Johannes Gutenberg University, Mainz

Calcium oxalate is the main component of kidney stones [1]. The presence of peptides such as poly-glutamate has a great impact on the crystalline phase, morphology and growth rate of calcium oxalate [2]. Understanding the biomineralization process and its inhibition requires a detailed microscopic characterization of the water/mineral and water/polymer/mineral interfaces. We performed Density Functional Theory (DFT) based Molecular dynamics simulations [3] to study the structure of the interfaces between Calcium Oxalate Dihydrate (COD) (100) and (101) / water. Our study reveals differences in the coordination of Calcium ions at the surface with water, which could be responsible for a different interaction with biopolymers. We also characterize the interaction between different surfaces of COD and biomolecules. As a first step we consider acetate as a model system containing a carboxylic group and we estimate its binding structure and free energies on different COD surfaces and for different concentration. Preferential binding of carboxylate to the 100 surface is found, therefore explaining recent experimental results on anisotropic growth of COD crystals in the presence of biopolymers [2]. [1] E. L. Prein and C. Frondel, J. Urol. 57, 949, 1947. [2] V. Fischer, K. Landfester and R. Munoz-Espi, Cryst. Growth Des. 11, 1880, 2011. [3] CP2K/QUICKSTEP, http://cp2k.berlios.de/

O 87.8 Fri 12:15 H31

Probing the interaction of ice nucleating proteins with water molecules using SFG spectroscopy — •Ravindra Pandey[1], Michael Schleeger[1], Janine Fröhlich[2], Ulrich Pöschl[2], Mischa Bonn[1], and Tobias Weidner[1] — [1]Max Planck Institute of Polymer Research, Mainz, Germany — [2]Max Planck Institute for Chemistry, Mainz, Germany

Specific Bacteria can cause crop frost damage by using ice-nucleating (IN) proteins anchored to their outer cell surfaces. IN proteins mimic the structure of ice surfaces and, thus, promote the growth of ice crystals by acting as efficient templates for ice nucleation. Frost damage caused by ice crystals facilitates bacterial invasion of affected plants. IN proteins not only play an important role for agriculture - airborne proteins can also promote ice formation in the atmosphere and may change precipitations patterns. The molecular mechanisms by which IN proteins interact with water molecules have not yet been resolved. We have investigated the interaction of IN proteins with water molecules using sum frequency generation (SFG) vibrational spectroscopy. When cooling the sample from room temperature to freezing, we found that the order of water molecules in contact with IN proteins is suddenly increased for temperatures near freezing (4-5°C). This effect was not observed for liquid water surfaces without the protein. The data also indicates a change of protein structure near the nucleation temperature.

O 87.9 Fri 12:30 H31

Quantitative Dissolution Rates of Active Pharmaceutical Molecules at the Crystal-Water-Interface from Molecular Dynamics Simulations — •Julian Schneider[1], Maximilian Greiner[2], Berna Dogan[1], Heiko Briesen[2], and Karsten Reuter[1] — [1]Department Chemie, Technical University Munich, Germany — [2]Chair for Process Systems Engineering, Technical University Munich, Germany

The dissolution of active pharmaceutical ingredients (API) plays a significant role in the pharmcokinetics of orally administered drugs. For the development of a fully-integrated in-silico multiscale approach to predict the dissolution rate of an API compound, detailed knowledge about the deintegration process of single molecules out of the crystal surface is required. Since a lot of prototypical API molecules, such as aspirin, do not exhibit spontaneous dissolution in the accessible time of atomistic molecular dynamics simulations, gathering such information turns out to be a difficult task. Employing advanced simulation techniques, we propose methods which allow for the accelerated simulation of molecular deintegration processes and the calculation of the associated rate constants. In a subsequent step these values can be used to couple the atomistic representation of the API-water-interface to a kinetic Monte Carlo (kMC) model in order to bridge the scale towards larger simulation times and systems.

O 87.10 Fri 12:45 H31

Electrochemical infrared spectroscopy to induce and detect neurotransmitter exchange across a solid-liquid interface — •Neelima Paul[1,3], Kenichi Ataka[2], Joachim Heberle[2], Peter Müller-Buschbaum[3], and Martha Ch. Lux-Steiner[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Freie Universität Berlin, Department of Physics, Experimental Molecular Biophysics, 14195 Berlin, Germany — [3]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85747 Garching, Germany

We present in-situ electrochemical-infrared spectroscopy data on voltage induced vibrational changes of neurotransmitter molecule, monosodium glutamate at a solid/liquid interface. For the polarised glutamate molecule, containing two deprotonated carboxylate groups and one protonated amine group at physiological pH, structural changes on application of different magnitudes of voltages at the solid electrode surface as well as molecular transfer events are resolved by surface-enhanced IR difference absorption spectroscopy (SEIDAS). Angular changes of bonds versus the surface normal have been determined because SEIDAS monitors only those vibrations whose dipole moment are oriented perpendicular to the solid surface. The application of positive and negative surface potentials (0.7 V) leads to the release of the glutamate molecules, which were initially adsorbed at the gold solid surface. This adsorption/release process is completely reversible. A possible application could be retinal implants.

O 88: Molecular Films

Time: Friday 10:30–12:45 Location: H38

O 88.1 Fri 10:30 H38

Chitosan conformation and its supramolecular complex with iodine on the silica surface — •Tetiana Podust, Tetiana Kulik, and Borys Palyanytsya — Chuiko Institute of Surface Chemistry of the NAS of Ukraine, 17 General Naumov str., Kyiv, 03164, Ukraine

Nowadays there are a lot of studies are focused on developing different strategies of nanomaterials surface functionalization with biopolymer. Such studies are of great interest for answering fundamental questions and for solving various practical tasks. Among other materials nanooxides modified with polysaccharides are promising systems due to their high potential for biotechnology, medicine, water treatment, engineering of eco-friendly materials etc. Consideration in this talk will be given to organic-inorganic hybrid nanomaterials based on silicas modified with chitosan. It is desirable to expand number of techniques which allow determining fraction of bound segments (p parameter) that is a key parameter for adsorbed polymer. A new approach based on the temperature-programmed desorption mass spectrometry (TPDMS) data for estimation of the p parameter of chitosan adsorbed on the silica will be proposed. It will be described main features of silicas surfaces modified with chitosan and iodine using a combination of FTIR and UV-vis spectroscopy, SEM, particle size analysis and thermogravimetry. A discussion about chitosan polymeric chains conformation on the silica surface and supramolecular inclusion complex of iodine with surface-immobilized polysaccharide will be given.

O 88.2 Fri 10:45 H38

Characterizing the protein-surface interactions that control diatom biomineralization — •Joe Baio[1], Adrienne Rohrig[2], Mischa Bonn[1], Gary Drobny[2], and Tobias Weidner[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]University of Washington, Seattle, WA 98195

The formation of silica-based cell walls in marine, single celled organisms, is regulated by protein-mineral interactions. The diatom species Cylindrotheca fusiformis assembles supermolecular silica structures via proteins called sillafins. In a silicic acid solution, specific repeat units within this protein, SSKKSGSYSGSKGSKRRIL (R5), induce the formation of silica-protein composite nanoparticles. The protein-surface interaction that drives self-assembly is likely controlled by specific contacts between the surface atoms and key protein side chains. In this study, we characterized this R5-SiO2 interaction by both near edge x-ray absorption fine structure (NEXAFS) spectroscopy and in situ sum frequency generation (SFG) spectroscopy. Two peaks within the amide I vibrational band of the SFG spectra, 1640 and 1670 cm-1, indicate that the R5 peptide retains a beta sheet conformation when interacting with SiO2. While details of the binding geometry of the single tyrosine within R5 is provided by the observed polarization dependence of the NEXAFS C1s to π^* transition related to the tyrosine's phenyl ring.

O 88.3 Fri 11:00 H38

self-assembled monolayers of partially fluorinated alkanethiols on gold and GaAs substrates — •Hao Lu[1], Andreas Terfort[2], and Michael Zharnikov[1] — [1]Applied Physical Chemistry, Heidelberg University, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — [2]Institute for Inorganic und Analytical Chemistry, Frankfurt University, Max-von-Laue-Straße 7, 60438 Frankfurt, Germany

Self-assembled monolayers (SAMs) of partially fluorinated alkanethiols (PFAT) gained substantial attention during past years because of their rigidity, oleophobicity, thermal stability, and potential use as nanoscale corrosion inhibitors. To better understand and use these properties it is important to obtain information on the structure and organization of the PFAT monolayers. In this context, we studied SAMs of a series of the PFAT molecules with the variable length of the fluorocarbon chain, viz. CF3(CF2)n(CH2)11SH (FnH11SH, n = 6, 8, and 10), on Au(111) and GaAs(001) by high resolution X-ray photoelectron spectroscopy, near edge X-ray absorption fine structure spectroscopy, and infrared reflection absorption spectroscopy. We demonstrate that FnH11SH form highly ordered and densely packed self-assembled monolayers on both these substrates, which is mediated by the thiolate-substrate bond. The orientational order is high on both Au and GaAs but deteriorates to some extent with the decreasing length of the fluorocarbon chain. This deterioration is more pronounced for GaAs which is intrinsically prone to degradation and oxidation and is, therefore, a quite sensitive substrate for molecular self-assembly.

O 88.4 Fri 11:15 H38

Modification of nitrile-terminated aromatic self-assembled monolayers by electron irradiation and related applications — Nikolaus Meyerbröker and •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, D-69120 Heidelberg, Germany

Here we describe the behavior of self-assembled monolayers (SAMs) of 4'-cyanobiphenyl-4-thiol (CBPT) on Au(111) upon electron irradiation. Under such a treatment, the aromatic framework of CBPT SAMs is laterally cross-linked while the nitrile groups, located at the SAM-ambience interface, are reduced to active amine moieties which can be used as docking sites for the coupling of other species. This makes CBPT monolayers as a promising system for conventional and chemical lithography as well as for nanofabrication. Along these lines, we demonstrate the preparation of complex polymer brushes, patterning of the underlying substrate, and fabrication of molecule-thin, freestanding membranes on the basis of CBPT SAMs. The balance between the application-favorable processes and defragmentation in these films is studied in detail and comparison to the well-established (for the relevant applications) system of 4'-nitrobiphenyl-4-thiols is performed. Taking CBPT SAMs as a model system, the effect of the energy of the primary electrons on the extent of the chemical transformation and cross-linking in substituted aromatic SAMs is investigated.

O 88.5 Fri 11:30 H38

Orientation and ordering in surface-bound DNA hybrids — Caitlin Howell[1], Yekkoni Lakshmanan Jeyachandran[2], Patrick Koelsch[1], and •Michael Zharnikov[2] — [1]Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Applied Physical Chemistry, University of Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

Films of surface-bound homo-oligonucleotides on gold were hybridized and characterized using x-ray photoelectron spectroscopy, near-edge x-ray absorption fine structure spectroscopy, and infrared reflection-absorption spectroscopy. First, the effect of rinsing after the hybridization step was studied. Further, the effects of target sequence mismatches and target length mismatches were investigated. The overall orientation of the probe and target strands was found to remaine upright and relatively unchanged despite the presence of up to four sequence mismatches in the target strands, although the total number of hybrids decreased with higher numbers of mismatches. Upright probes were also observed in hybrids formed with targets of shorter length, with a greater number of hybrids present in these films as compared to those formed with longer targets. These results suggest that in DNA films of relatively high densities, such as those tested here, the presence of sequence or length mismatches in target strands does not result in a large disruption of orientation and ordering in surface-bound hybrids. This finding may be useful for nanotechnological applications or utilization of DNA microarrays for biosensing purposes.

O 88.6 Fri 11:45 H38

Thermal Influence on the Structure of Alkylsiloxane Monolayers examined by SFG-Spectroscopy — •Jan Weber, Thorsten Balgar, and Eckart Hasselbrink — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

As organic monolayers have very diverse characteristics they offer an interesting field of surface science. Especially alkylsiloxane monolayers are of interest because of their potential for modifying surfaces. Promising applications include wetting, fine-scale lithography or protection of metals against corrosion.

Alkylsiloxanes are known to form self-assembled monolayers (SAMs) that are stable under ambient conditions. Since many applications require compatibility with heating it is our goal to get a better understanding of alkylsiloxane SAMs on a molecular level at elevated temperature.

In this study we apply vibrational sum-frequency generation (SFG) spectroscopy to an octadecylsiloxane (ODS) monolayer on a glass substrate using a picosecond laser system. This method is particularly suitable because its selective surface sensitivity. Our results are discussed with respect to temperature dependent chain disorder and orientation on the surface.

O 88.7 Fri 12:00 H38

Confinement of electrons in metal-coordinated and covalently bonded two dimensional nanoporous molecular networks — •Aneliia Shchyrba[1], Susanne Martens[1], Christian Wäckerlin[2], Toni Ivas[1], Jorge Lobo-Checa[3], Manfred Matena[4], Lutz H. Gade[5], Meike Stöhr[6], and Thomas A. Jung[2] — [1]University of Basel, Switzerland — [2]Paul Scherrer Institut, Switzerland — [3]Spanish National Research Council (CSIC), Spain — [4]Donostia International Physics Center (DIPC), Spain — [5]Universität Heidelberg, Germany — [6]University of Groningen, Netherlands

Two dimensional (2D) nanoporous networks are intensively studied for their capability to act as quantum wells confining the surface state of a suitable substrate like Cu(111) or for the study of host-guest assemblies. Structures which are stabilized by strong interactions (i.e. by metal-coordination or by covalent bond-formation) are of special interest as they are more stable and therefore better suited to host strongly interacting guest molecules without collapse, up to elevated temperatures. Herein, we review the strictly regular, hexagonal DPDI (4,9-diaminoperylene-quinone-3,10-diimine) network which is based on metal-coordination to proceed towards novel, irregular 2D nanopores based on covalent bond-formation. While the former allows even to observe the confined surface state by spatially averaging, angle-resolved photoemission since the same confinement is repeated over-and-over, the irregular pores are observed to lead to a whole collection of differently sized and shaped quantum wells.

O 88.8 Fri 12:15 H38

High Resolution Core-Level Spectroscopy of Molecular Switches at Silicon(111) Surfaces — •Daniel Przyrembel[1], Michael Åxman Petersen[2], Andreas Hebert[2], Karola Rück-

Braun[2], and Martin Weinelt[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin — [2]Institut für Chemie, Technische Universität Berlin

Si(111) surfaces, functionalised with organic molecular switches of the fulgimide[1] and dihydroazulene[2] (DHA) type, have been investigated by means of high resolution X-ray photoelectron spectroscopy (XPS). The versatile anchoring strategy involves first the attachment of alkyl acid chains to the H-terminated Si(111) single crystal surface and second coupling of the molecular switches to these carboxyl linkers. This leads to very stable and durable self assembled monolayers (SAMs). The linker chain-density can be adjusted by mixing in inert alkyl chains. Thus the packing density of molecular switches becomes tuneable. All steps of the sample preparation have been monitored and their efficiency proven. Fulgimides are optically switchable between open and closed forms by irradiation with UV and visible light, DHA turns into its isomer vinyl heptafulvene (VHF) upon optical stimulation and reacts back thermally. The reversible switching of the molecules leads to small, reproducible modifications of the XP spectra, *i.e.* peak shifts and shape changes, only weakly affected by successive beam damage. A reduced packing density of molecular switches improves the switching efficiency. [1] Y. Yokoyama *Chem. Rev.* **2000**, *100*, 1717-1739; [2] J. Daub, T. Knöchel, A. Mannschreck *Angew. Chem.* **1984**, *96*, 980-981

O 88.9 Fri 12:30 H38

Determining excitation pathways in a hybrid metal-organic interface state using coherent 2D nanoscopy — M. Aeschlimann[1], T. Brixner[2], M. Cinchetti[1], N. Grossmann[1], M. Hensen[3], C. Kramer[2], P. Melchior[1], W. Pfeiffer[3], M. Piecuch[1], C. Schneider[1], S. Steil[1], C. Strüber[3], and •P. Thielen[1,4] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [4]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany

Coherent 2D nanoscopy combines the principle of conventional 2D spectroscopy with photoemission electron microscopy (PEEM). While 2D spectra are well suited for studying the dynamics of quantum states as well as interactions between them, PEEM allows for detection of the electrical near field of nano-structured samples with a resolution beyond the optical diffraction limit. We use coherent 2D nanoscopy to study the hybrid electronic state forming at the interface between cobalt and the organometallic complex tris(8-hydroxyquinolinato)aluminium (Alq3). We observe the excitation paths at such a hybrid metal-organic interface and monitor the subsequent electron dynamics in the hybrid interface state. The lateral resolution enables us to address small ensembles of quantum systems rather than large-scale averaging.

O 89: Surface Dynamics II

Time: Friday 10:30–13:15 Location: H33

O 89.1 Fri 10:30 H33

Spin polarized photoemission of gold surfaces coated with bacteriorhodopsin — •Matthias Kettner[1], Benjamin Göhler[1], Tal Z. Markus[2], Volker Hamelbeck[1], Georg F. Hanne[1], Ron Naaman[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Chemical Physics, Weizmann Institute, Rehovot, Israel

Electron spin polarization has been measured for photoelectrons emitted from a gold substrate and transmitted through physisorbed layers of the chiral membrane protein bacteriorhodopsin. Samples are irradiated by circularly as well as linearly polarized 213 nm laser radiation, exciting photoelectrons within the gold substrate which are transmitted through the proteins. Photoelectrons are analyzed by a time-of-flight detector yielding an "unstructured" spectrum up to 1.5 eV; an electron dichroism of up to 1.4 % is measured independent on the kinetic energy. Furthermore, a Mott polarimeter is used for spin analysis. In the present experiment electron spin polarization values of up to 15 % are obtained independent of the polarization of the incident light, similar to earlier work on ordered layers of double-stranded oligo-DNA [1]. The measured electron spin polarization shows a dependence on the preparation of the samples.

[1] B. Göhler, et al., Science 331, 894 (2011)

O 89.2 Fri 10:45 H33

Tight-binding spin dynamics and tight-binding Monte Carlo: a study on BCC iron — •Siebe Rossen[1,2], Phivos Mavropoulos[1], Timo Schena[1], Stefan Blügel[1], and Theo Rasing[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Radboud Universiteit Nijmegen, Institute for Molecules and Materials, 6525AJ Nijmegen, The Netherlands

Recent laser pulse excitation experiments on metallic films [1] show remarkable magnetisation dynamics which call for a theoretical explanation on an atomistic scale. So far the computational approach to this problem has been primarily based on a Heisenberg Hamiltonian at best, the validity of which becomes questionable in strongly noncollinear magnetic states. Therefore, we developed a code based on a calculation of the time-dependent electronic structure within the tight-binding and adiabatic approximation, in which the torque acting on the individual moments can be obtained in any spin configuration outside equilibrium. Such a method, for which the underlying principles are given in [2], is not only powerful because of the accurate description of the dynamics of magnetic materials based on the integration of the equation of motion [3], but it can also provide insights in thermodynamic properties of magnetic systems when incorporated into a Monte Carlo scheme. We will show results for BCC iron. The authors thank the Fantomas project for funding. [1] A. Kirilyuk *et al.*, RMP **82**, 2731 (2010). [2] M.V. You and V. Heine, JPF: Met. Phys. **12**, 177 (1982). [3] P. Ma and S.L. Dudarev, PRB **86**, 054416 (2012).

O 89.3 Fri 11:00 H33

Emission of correlated positron-electron pairs from surfaces — •Iuri Stefani Brandt[1], Zheng Wei[1], Frank Oliver Schumann[1], and Jürgen Kirschner[1,2] — [1]Max-PlanckInstitut für Mikrostrukturphysik, Halle, Germany — [2]Martin-LutherUniversität, Halle, Germany

The electron correlation is due to the combined action of the Pauli principle and Coulomb interaction. Electron pair emission is a powerful tool to study the aspects of the electron correlation. One way to disentangle the Pauli principle from the Coulomb interaction is to explore correlated positron-electron pair emission upon primary positron impact. This process of positron-electron pair emission is detectable and motivated a theoretical study [1,2]. We developed a dedicated laboratory positron source employing a Na22 isotope which provides a flux of 4x10^4 e$^+$/s for kinetic energies in the range of 40-70 eV. We employ a symmetric geometry in which the incoming positrons hit the target along the surface normal. The emitted particles are measured in coincidence via a pair of energy dispersive spectrometers. We investigated NiO/Ag(100) and Ag(100) surfaces. In the case of electron pair emission upon primary electron impact we observe a symmetric two-dimensional energy distribution, because electrons are not distinguishable. Contrary to this electrons and positrons are distinguishable leading to an asymmetric two-dimensional energy distribution.

[1] G.A. van Riessen et al., JPCM **20**, 442001 (2008).
[2] F. Giebels et al., JPCM **21**, 355002 (2009).

O 89.4 Fri 11:15 H33

Space-Charge Interaction in Electron Momentum Microscopy — •Gerd Schönhense[1], Katerina Medjanik[1], Marieke de Loos[2], and Bas van der Geer[2] — [1]Institut für Physik, Uni. Mainz, Germany — [2]Pulsar Physics, Eindhoven, The Netherlands

Ultrahigh-brightness sources like (X)FELs, but also table-top higher harmonics sources offer fascinating experimental possibilities. Unfortunately, electron spectroscopic methods like photo- or Auger-electron spectroscopy at such sources are facing a dramatic loss in performance due to the space-charge problem. Coulomb interaction in the beam can induce prohibitively large energy broadenings ΔE of hundreds to thousands of eV. We have considered the space-charge effect for the special situation of a momentum microscope in the hard X-ray range, based on simulations with the General Particle Tracer (GPT) code. We find that momentum microscopy offers a pathway for a certain space-charge correction since the instrument detects the $k_{||}$- distribution in a parallel-imaging microscope column. For XFEL applications in the hard X-ray range a strong immersion field of 5 MV/m (close to the limit of potential breakthrough) accelerates and widens the electron beam very rapidly, in order to reduce Coulomb repulsion. The correction makes use of the fact that the line of best-fit of the electron distribution in an energy-vs-radius plot appears tilted and can be used for a re-normalization of the measured kinetic energies. GPT calculations for different model distributions including the intense low-energy signal from the secondary cascade reveal chances of a possible space-charge correction approach. Project funded by BMBF (05K12UM2).

O 89.5 Fri 11:30 H33

Femtosecond time-resolved photoemission on 1*T*-TaS$_2$ in the Mott-insulating state — •Isabella Avigo[1], Simon Freutel[1], Laurenz Rettig[1], Manuel Ligges[1], Lutz Kipp[2], Kai Rossnagel[2], and Uwe Bovensiepen[1] — [1](1)*Universität Duisburg-Essen, D 47048 Duisburg — [2](2)*Christian-Albrechts-Universität zu Kiel, D 24118 Kiel

1*T*-TaS$_2$ is a quasi-two-dimensional transition metal dichalcogenide undergoing a metal-to-insulator transition below 180 K in which a charge density wave (CDW) coexists with a Mott insulating state. Of particular interest is the photoinduced melting of the Mott-Hubbard phase which drives the system in a crossover state [1,2] substantially different from the high temperature metallic state. Femtosecond time- and angle-resolved photoemission measurements were performed in the Mott-insulating phase at different pump fluences from 0.1 to 1 mJ/cm^2. We observe a population of states above the Fermi level (E_F) after pumping and a depletion and broadening of the lower Hubbard band (LHB) peak below E_F. Our analysis reveals a difference in the relaxation dynamics of the electron population above E_F, which decays in about 350 fs, and the intensity of the lower Hubbard band, recovering in about 900 fs. This points to a possible decoupling of populations above and below E_F and thus to an at least unconventional metallic behavior in the photoinduced state.

We acknowledge support by the DFG through BO 1823/2, /4 and the EU under grant agreement 280555 within FP7. [1] Perfetti et al., NJP 10, 053019 (2008) [2] Dean et al., PRL 106, 016401 (2011)

O 89.6 Fri 11:45 H33

Long lived electrons trapped in amorphous ice adsorbed on Cu(111) — •Daniel Wegkamp, Michael Meyer, Clemens Richter, Julia Stähler, and Martin Wolf — Fritz-Haber-Institute of the MPG, Dep. of Physical Chemistry, Berlin

In polar environments excess charges are stabilized by reorientation of the surrounding dipoles. We have studied the trapping of excess electrons and their subsequent dynamics in amorphous solid water (ASW) adsorbed on a Cu(111) surface. The electrons are excited in the metal with ultraviolet (UV) femtosecond laser pulses and injected into 20 to 35 bilayer (BL) thick ASW layers. Their stabilization and relaxation dynamics are probed by time-resolved photoemission spectroscopy. In contrast to previous studies on thin (< 7 BL) ASW layers where subpicosecond lifetimes have been reported [1] we observe 14 orders of magnitude longer lifetimes. These electrons reside in an excited state between 2 and 3 eV above the metal's Fermi level for tens of seconds. The binding sites of the trapped electrons are located at the ice-vacuum interface, as their spectroscopic signature is affected strongly by a co-adsorbed Xe-overlayer. Furthermore, we have studied the changes of workfunction and occupied electronic structure induced by UV irradiation and discuss possible origins.

[1] J. Stähler et al., Chem. Soc. Rev. 37 (2008) 2180

O 89.7 Fri 12:00 H33

Electron Traps at the Ice Surface — •Michel Bockstedte and Anja Michl — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudstr. 7B2, D-91058 Erlangen

Water, water clusters and ice possess the fascinating ability to solvate electrons. On the surfaces of water clusters[1] and thin crystalline ice layers deposited on a metal substrate[2] long-living solvated electron states were observed that evolve from pre-existing surface traps. The identification of initial electron traps provides important insight into the electronic structure of the water surface, ice layers on metals and the dissociative interaction of electrons with adsorbates. Theoretical models[2] based on the bilayer terminated Ih-(0001) surface related such traps to orientational defects or vacancies with dangling OH-groups.[3] So far, a conclusive microscopic model of the electron traps at the surface of water structures on metals is missing. Here we address such electron traps including also water ad-structures observed by STM[4] theoretically using hybrid density functional theory and many-body perturbation theory in the G$_0$W$_0$ approximation. We identify a hierachy of traps with increasing vertical electron affinity, ranging from water admolecules and hexagon adrows via clusters of orientational defects to vacancy-related traps.

[1] Siefermann and Abel, Angew. Chem. Int. Ed. 50, 5264 (2011).
[2] Bovensiepen et al., J. Chem. Phys. C **113**, 979 (2009).
[3] Hermann et al., J. Phys. Condens. Matter **20**, 225003 (2008).
[4] Mehlhorn and Morgenstern, Phys. Rev. Lett. **99**, 246101 (2007).

O 89.8 Fri 12:15 H33

Improving the Temporal Resolution of a Time Resolved Electron Diffraction Experiment with Tilted Laser Pulse Fronts — •Annika Kalus, Carla Streubühr, Tim Frigge, Anja Hanisch-Blicharski, Boris Krenzer, Manuel Ligges, Ping Zhou, Uwe Bovensiepen, Dietrich von der Linde, and Michael Horn-von Hoegen — Universität Duisburg-Essen, Fakultät für Physik und Center for Nanointegration Duisburg-Essen (CENIDE)

Time resolved reflection high energy electron diffraction (RHEED) is an ideal tool to study the response of the surface lattice upon femtosecond laser pulse excitation. To achieve ps time resolution a laser pulse is used in a pump probe setup to excite the sample and to generate an electron pulse via photoemission that probes the sample. The temporal resolution of the experiment is limited by the velocity mismatch between laser pump pulse and the probing electron pulse at grazing incidence. To compensate this mismatch we realized an optical setup to tilt the laser pulse front by 70° in order to achieve temporal and spatial overlap with the 30 keV electron pulse over the entire width of the sample. The tilted laser pulse was characterized by a cross-correlator based on second harmonic generation.

Using the thermal response of thin Pb films on Si(111) upon laser excitation we optimized the optical setup and determined an improved temporal resolution of less than 1.8 ps at 29 keV electron energy. Electron phonon coupling in Bi is much weaker and results in a slow down of the heating of thin Bi films: a time constant for the excitation of about 10 ps was observed.

O 89.9 Fri 12:30 H33

2PPE-measurement with an angle-resolving time-of-flight spectrometer — •Thomas Kunze[1,2], Dominic Lawrenz[1], Jens Kopprasch[1], Martin Teichmann[1], Thorsten U. Kampen[2], and Martin Weinelt[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]SPECS GmbH, Berlin, Germany

To increase the efficiency of electronic structure measurements we developed in cooperation with SPECS an angle-resolving time-of-flight spectrometer.

The instrument allows to measure the kinetic electron energy as a function of the two-dimensional parallel crystal momentum (E vs. $k_{x\|}$ and $k_{y\|}$) without rotating the sample. The electron lens in front of the detector allows angle or spacial resolved measurements.

While developing this new machine a number of issues had to be addressed. We developed a proper way to simulate the electron trajectories, found a method to suppress secondary electrons and established a suitable measurement procedure. The use of the instrument is not as common as measurements with a hemispherical analyzer. We will point out the advantages and disadvantages of the method.

The talk will cover the alignment of the spectrometer itself and relative to the sample and the working principle of the detector gating unit.

Finally, we will report on our two-photon photoemission studies of Cu(111) and Cu(1 1 11) which illustrate the potential of time-of-flight electron spectroscopy.

O 89.10 Fri 12:45 H33

Comparison of the electronic surface states of Si(100) and Ge(100) studied by 2PPE — Kristof Zielke, •Jens Kopprasch, Christian Eickhoff, Cornelius Gahl, and Martin Weinelt — Fachbereich Physik der Freien Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We have investigated the electronic surface states at the (100)-surfaces of Si and Ge, two of the most important semiconductor surfaces in the device industry. Si(100) and Ge(100) are ideal for a comparison, because they have the same crystal structure and surface reconstruction, but exhibit distinct bulk band structures. We discuss the binding energy, the dispersion and the lifetimes of the dangling-bond states and the image-potential resonances on both surfaces and address the excitation of these surface states and their coupling to valence and conduction band continua. Furthermore, we show that the decay of photo-excited electrons in the conduction band is significantly influenced by the surfaces states. In particular, we discuss the role of inter- and intraband electron-phonon scattering between the conduction band and the unoccupied surface state D_{down}, and back scattering to the valence band. Thereby we found significant differences in the timescale of the decay processes on Si and Ge.

O 89.11 Fri 13:00 H33

Mono-energetic target surface electron (TSE) beams produced via surface guiding and acceleration in femtosecond laser-solid interactions — •Jingyi Mao[1], Liming Chen[2], Xulei Ge[2], Lu Zhang[2], Wenchao Yan[2], Dazhang Li[3], Guoqian Liao[2], Jinglong Ma[2], Kai Huang[2], Yutong Li[2], Xin Lu[2], Quanli Dong[2], Zhiyi Wei[2], Zhengming Sheng[2], and Jie Zhang[2,4] — [1]TU Kaiserslautern and Research Center OPTIMAS, 67663 Kaiserslautern, Germany — [2]Beijing National Laboratory of Condensed Matter Physics, Institute of Physics, CAS, Beijing 100190, China — [3]Institute of High Energy Physics, CAS, Beijing 100049, China — [4]Department of Physics, Shanghai Jiao tong University, Shanghai 200240, China

Highly collimated MeV TSE guiding has been observed along the target surface following the interaction of bulk target irradiation by femtosecond laser pulses at relativistic intensities[1]. The beam quality is shown to depend critically on the laser contrast: with a ns prepulse, the generated electron beam is well concentrated and intense, while high laser contrast produces divergent electron beams. In the case of large preplasma scale lengths on the target surface, tunable guiding and acceleration of TSE is achieved by changing the laser incident angle. By expanding the preplasma scale length to several hundred micrometers, we obtained MeV monoenergetic TSE beam with 100 pC per laser pulse and divergence angles of only 3 degrees, which could be used as a stable injector for accelerators.

[1] J. Y. Mao et al., Phys. Rev. E. 85, 025401(R)(2012)

O 90: Semiconductor Substrates

Time: Friday 10:30–13:15 Location: H45

O 90.1 Fri 10:30 H45

Growth Study of Thin MgO Films on Fe(001) — •Hendrik Ronneburg, Stefanie Stuckenholz, Christin Büchner, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

The electronic structure and morphology of oxide surfaces are of crucial importance for their reaction behaviour. A detailed understanding of the structure-reactivity relationship is desired for the studies in heterogeneous catalysis.

We use noncontact atomic force microscopy (nc-AFM) and scanning tunneling microscopy (STM) to study model catalysts, namely metal supported thin oxide film systems.

Thin MgO films can be grown on different metal substrates, e.g. Mo(001), Ag(001) or Fe(001). MgO films grown on Mo(001) and on Ag(001) have been studied in detail by scanning probe methods [1, 2]. The electronic structure and morpholgy of the oxide film is altered by the substrate. To further investigate this support influence on the properties of thin oxide films our present studies focus on the system of MgO grown on Fe(001).

Here we present preliminary results from our growth study of thin MgO films on Fe(100).

[1] S. Benedetti, *et al.*, Chem. Phys. Lett. **430**, 330 (2006)
[2] T. König, *et al.*, J. Phys. Chem. C **113**, 11201 (2009)

O 90.2 Fri 10:45 H45

Concentration of point defects at metal-oxide surfaces: case study of MgO (100) — Norina A. Richter[1], Sabrina Sicolo[2], •Sergey V. Levchenko[1], Joachim Sauer[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem 14195, Germany — [2]Humboldt-Universität zu Berlin, Berlin 10099, Germany

We calculate from first principles the concentration of neutral and charged oxygen vacancies on a doped MgO (100) surface at realistic (T, p_{O_2}) conditions. Vacancy formation energies are computed using hybrid density-functional theory with parameters of the exchange-correlation functional adjusted according to a basic consistency requirement on the Kohn-Sham and G_0W_0 defect transition levels. The parameters are validated by CCSD(T) calculations of formation energies for neutral vacancies using embedded cluster models. Gibbs free energies of formation are obtained using the *ab initio* atomistic thermodynamics approach [1]. We demonstrate that the concentration of surface vacancies is significantly increased due to band bending and Fermi level pinning at the surface, resulting in lower formation energies of charged vacancies.

[1] K. Reuter and M. Scheffler, Phys. Rev. B **65**, 035406 (2001); C. M. Weinert and M. Scheffler, Mat. Sci. Forum **10-12**, 25 (1986); M. Scheffler and J. Dabrowski, Phil. Mag. A **58**, 107 (1988).

O 90.3 Fri 11:00 H45

Ultra-thin ZnO films on metal substrates from first principle — •Bjoern Bieniek, Yong Xu, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

In the context of catalysis and hybrid inorganic/organic systems, metal supported ultra-thin ZnO films can be used to model catalysts or ZnO surfaces. By means of density-functional theory (DFT - PBE and the hybrid functional HSE) we investigate the structure of ultra-thin ZnO on the (111) surfaces of Ag, Cu, Pd and Pt. In contrast to the bulk, the free-standing ZnO mono-layer adopts a graphene-like structure [1]. We find that this flat structure prevails on the metal substrates and obtain coincidence structures in good agreement with experiment [2, 3]. The influence of O_2 and H_2 environments is investigated with ab-initio thermo-dynamics [4] and surface phase diagrams are presented. Zn- and O-point defects are stabilized in the mono-layer by the substrates that would not be present in the freestanding ZnO mono-layer. With decreasing nobility of the metal substrate, the stability of defects, in particular inter-facial O, increases and the corrugation of the film becomes more pronounced. With increasing H_2 partial pressure sparse ring structures occur in Zn poor conditions. Metal supported ultra-thin ZnO films therefore do not resemble conventional ZnO surfaces and should be regarded as distinct nano-systems in their own right. [1] Z. C. Tu and X. Hu, PRL **94**, 035434 (2006) [2] C. Tusche *et al.* PRL **99**, 026102 (2007) [3] G. Weirum *et al.* J. Phys. Chem. C, 114 (2010) [4] K. Reuter and M. Scheffler, PRB **68**, 045407 (2003)

O 90.4 Fri 11:15 H45

Manipulation of subsurface donors in ZnO — •hao zheng, alexander weismann, and richard berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

The capability of manipulating structures at the atomic scale has become an important asset of the scanning tunneling microscope (STM). Nowadays atoms may be arranged into nanostructures with device-like functions. Usually this exquisit control is limited to adatoms. A recent exception is interstitial H in Pd, which could be moved with an STM tip. No comparable results have been reported for semiconductors where the controlled positioning of individual dopants would be desirable. We present the manipulation of interstitial Zn in ZnO, a semiconductor with extraordinary properties. Zn interstitials are of particular interest because they may be the sought-after shallow donors that lead to n-type conductance of ZnO despite its wide band gap of 3.4 eV.

O 90.5 Fri 11:30 H45

Cyclooctyne adsorption on clean and hydrogen precovered Si(001) surfaces — •Gerson Mette[1], Michael Dürr[1,2], Ruben Bartholomäus[3], Ulrich Koert[3], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — [2]Fakultät Angewandte Naturwissenschaften, Hochschule Esslingen, D-73728 Esslingen —

[3]Fachbereich Chemie, Philipps-Universität, D-35032 Marburg

The reaction of organic adsorbates on semiconductor surfaces is of special interest with respect to surface functionalization and its use in molecular electronics. Whereas several alkenes and alkynes exhibit well ordered monolayers on Si(001), second- and multilayer attachment is still a central challenge towards successful functionalization.

In this context, the adsorption of cyclooctyne on clean and hydrogen precovered Si(001) surfaces was investigated by means of STM. The adsorption behavior was observed to be similar at room temperature and at low surface temperature of 50 K in contrast to systems like C_2H_4/Si which adsorb via a mobile precursor state. Moreover, it was found to be insensitive to distorted, hydrogen-induced dangling-bond configurations. At high coverage, cyclooctyne forms well ordered structures on Si(001). Our results suggest a direct adsorption pathway for cyclooctyne on Si(001) most likely governed by the molecule's triple bond in combination with its high ringstrain. This should make cyclooctyne a good candidate for chemoselective cycloadditions in more complex multifunctional compounds.

O 90.6 Fri 11:45 H45

Self-assembly of cis-Oligodiacetylenes from solution — •Christian Steiner[1], Erin T. Chernick[2], David Gessner[1], Maximilian Ammon[1], Rik R. Tykwinski[2], and Sabine Maier[1] — [1]Department of Physics, University of Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen, Germany — [2]Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Henkestraße 42, 91054 Erlangen, Germany

Cis-Oligodiacetylenes (ODAs) typically tend to adopt a folded, helical conformation in solution. Helical oligomers or polymers with a conjugated, chiral backbone provide a material with unique electronic and photonic properties which can be applied towards enantioselective sensing, chiral catalysis or for templating self-assembly, yielding chiral nanostructures.

The influence of the solvent on the conformation of ODAs was probed both by scanning tunneling microscopy and atomic force microscopy in ambient condition. We found that molecules solved in isopropanol aggregate in clusters, while molecules solved in tetrahydrofuran form flat films on the surface. Clusters on Mica surfaces are typically larger than on HOPG indicating that not only the solvent but also the surface charge influences the aggregation of the molecules. Molecularly resolved scanning tunneling microscopy images on HOPG suggest that in films the ODAs assemble in wire-like structures.

O 90.7 Fri 12:00 H45

The interface of III-V semiconductors to H_2O studied by reflection anisotropy spectroscopy and UPS — •Wolf-Dietrich Zabka[1,2], Matthias M. May[1,2], Oliver Supplie[1,2], Helena Stange[1,2], Christian Höhn[1], Hans-Joachim Lewerenz[1,3], and Thomas Hannappel[1,4,5] — [1]Helmholtz-Zentrum Berlin, Institute for Solar Fuels — [2]Humboldt-Universität zu Berlin, Institut für Physik — [3]California Institute of Technology, Pasadena, USA — [4]Technische Universität Ilmenau, Institut für Physik,Fachgebiet Photovoltaik — [5]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

III-V semiconductors are a promising absorber material class for solar-driven water splitting [1]. The interface between the semiconductor and H_2O is crucial for stability as well as charge transfer efficiency to the electrolyte [2,3].

For a better understanding of this interface, we perform model-experiments applying H_2O-adsorption in UHV to the surface of GaP(100) and InP(100) prepared by metalorganic vapour phase epitaxy (MOVPE). The influence of adsorbed water on III- and V-rich surfaces was examined with reflection anisotropy spectroscopy (RAS) and ultraviolet photoelectron spectroscopy (UPS). The two surface terminations show substantially different responses to H_2O. A comparison to results for UHV-cleaved surfaces [3] tries to illuminate the role of hydrogen-termination for these MOVPE-prepared surfaces.

[1] H. Döscher et al., *ChemPhysChem* **13**: 2899 (2012); [2] B. Wood et al., *The Journal of Chemical Physics* **136**: 064705 (2012); [3] O. Henrion et al., *Surface Science* **457**: L337 (2000).

O 90.8 Fri 12:15 H45

STM Observation of Krypton Adsorbed on Graphite — •Raphael Bindel, Tomohiro Matsui, and Hiroshi Fukuyama — Department of Physics, Graduate School of Science, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

Physisorption of a Krypton monolayer on graphite in the $\sqrt{3}x\sqrt{3}R30$ commensurate phase is investigated by low-temperature scanning tunneling microscopy (STM) at $T<100\,\mathrm{mK}$. Former experiments have shown the visibility of Krypton on Graphite in STM images [1]. We observe the growth of the Kr monolayer directly. Moreover, the Krypton adsorption site is determined to be the hollow site of the Carbon lattice by using the lateral boundary between Graphite and islands of the Krypton commensurate phase. In partial agreement with density functional theory calculations [1], the $4p$ and $5s$-states of the Krypton atoms appeared in STM images recorded at different voltages for the occupied as well as for the unoccupied states.

O 90.9 Fri 12:30 H45

Formation of Lu silicide on Si (111)-7x7 surface: STM/PES study at room temperature and low coverage — •Pavel Shukrynau[1], Xu Ying[1], Lars Smykalla[1], Martin Vondracek[2], and Michael Hietschold[1] — [1]Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group. D-09107 Chemnitz, Germany — [2]Institute of Physics Academy of Sciences of the Czech Republic, Cukrovarnická 10. CZ 162 53 Prague, Czech Republic

Interaction of very small amounts of lutetium with Si (111)-7x7 reconstructed surface was investigated in detail using combination of Scanning Tunneling Microscopy/Spectroscopy and Photoelectron Spectroscopy. Two distinct types of nanoclusters were found in the initial growth of the Lu/Si interface: the clusters of the first type have well defined globular shape with the average size of about 1 nm and are tightly bound to the underlying substrate. Other type of clusters is not homogeneous, showing a motion inside one half of the 7x7-unit cell. Analysis of photoelectron spectra of the Si 2p core levels shows core level binding energy shifts and intensity variations of Si surface related components, which clearly indicate that the reaction starts already at room temperature. Comparison of tunneling spectra with valence band PES data allows to determine the electronic structure of adsorbed species locally and suggests the formation of Lu-rich silicide.

O 90.10 Fri 12:45 H45

AlGaN/GaN based pH-sensitive field-effect transistors for nonaqueous solutions — •Johannes Anzt[1], Volker Cimalla[1], Wilfried Pletschen[1], and Oliver Ambacher[1,2] — [1]Fraunhofer Institute for Applied Solid State Physics, Freiburg, Germany — [2]Laboratory for Compound Semiconductor Microsystems, University of Freiburg, Germany

The purpose of this work is to characterize ion-sensitive field effect transistors (ISFETs) based on AlGaN/GaN heterostructures for measurements in nonaqueous solutions. For example, organic solvents offer larger potential windows for electrochemical techniques. Moreover, the pH value in biofuel is an important parameter to characterize quality. While ISFET sensors have already shown excellent sensing properties in aqueous solutions, pH measurements in nonaqueous solutions are faced to several challenging obstacles. Nonaqueous solutions often have low conductivity and the preparation of buffer solutions can be limited by solubility of the constituents. By definition, pH-scales in different solvents or solvent mixtures are not equal, thus, their pH-values ($\mathrm{pH} = -\lg a(\mathrm{H}^+)$) are not comparable. For example, reactivity at pH = 0 in liquid ammonia is by far lower than at pH = 0 in acetic acid. As the pH-ISFET response directly depends on the surface potential, which in turn is directly related to the activity of protons, it offers a possibility to get a universal measuring device with an alternative universal pH-scale.

O 90.11 Fri 13:00 H45

Heteroepitaxial growth of GaP on Si(111) substrates for III-V nanowire solar cells — •Agnieszka Paszuk[1,2], Weihong Zhao[1,2], Matthias Steidl[1,2], Sebastian Brückner[1,2], Anja Dobrich[2], Johannes Luczak[2], Peter Kleinschmidt[2,3], Henning Döscher[1,2], and Thomas Hannappel[1,3] — [1]Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, Ilmenau — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, Erfurt

III-V nanowires provide opportunities to realize high efficiency solar cells. We intend to grow nanowires by metal organic vapor phase epitaxy (MOVPE) on III-V/Si(111) templates to benefit from silicon as a low cost substrate. As a buffer layer we use GaP, since it is almost lattice matched to silicon. To achieve successful nanowire growth on GaP/Si(111) it is required to prepare GaP(111)B surfaces. A contamination-free transfer system enables us to study the MOVPE prepared surfaces with various surface science tools. To understand the heteroepitaxial growth of GaP on Si(111) we studied homoepitaxial GaP(111)A and B surfaces as a reference. Different characteristic surface reconstructions visible in low energy electron diffraction (LEED) enable identification of the GaP polarity. For growth on Si(111), changing the Si surface termination we can control the resulting GaP polarity.

O 91: Graphene: Preparation and Characterization II (jointly with HL, MA and TT)

Time: Friday 10:30–13:00 Location: H17

O 91.1 Fri 10:30 H17

Engineering of 2D-Nanomaterials by Swift Heavy Ion Irradiation — •Oliver Ochedowski, Hanna Bukowska, Sevilay Akcöltekin, and Marika Schleberger — Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg

Two dimensional (2D) nanomaterials prepared from layered crystal materials have attracted a great amount of interest in multiple fields of science. These nanomaterials can be metallic (e.g. graphene), semiconducting (MoS2) or insulating (Mica) with properties often different from their bulk counterparts. Here, we will demonstrate how the morphology of several 2D-nanomaterials can be modified by swift heavy ion (SHI) irradiation in the MeV regime under glancing incidence angle. The induced modifications are investigated by means of atomic force microscopy. In the case of graphene we will show by Kelvin probe force microscopy how SHIs can be used to alter the electronic structure and induce doping of the graphene.

O 91.2 Fri 10:45 H17

Fabrication of laterally structured graphene/carbon nanomembrane hybrids — •Andreas Winter[1], Stefan Wundrack[2], Rainer Stosch[2], and Andrey Turchanin[1] — [1]Universität Bielefeld, 33615 Bielefeld — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig

Laterally structured free-standing micro- and nanostructures of single-layer graphene (SLG) embedded into dielectric sheets with a thickness comparable to graphene are of great interest for applications in electronic or optoelectronic devices. However, their fabrication is not a trivial task at present. Here, we demonstrate how such hybrids can be engineered using electron-irradiation-induced crosslinking of graphene micro-/nanostructures with carbon nanomembranes (CNMs). CNMs are a dielectric 2D carbon material with the thickness of about 1 nm consisting of cross-linked randomly oriented benzene rings. We show scalable production of well-defined laterally patterned CNM-SLG hybrids of various architectures and characterize their structural, chemical and electronic quality by complementary spectroscopic and microscopic techniques including helium ion microscopy and Raman spectroscopy. Application areas of the generated hybrids will be discussed.

O 91.3 Fri 11:00 H17

Non-destructive chemical functionalization of single-layer graphene for electronic applications — Mirosław Woszczyna[1], Miriam Grothe[1], Andreas Winter[2], Annika Willunat[1], Stefan Wundrack[1], Rainer Srosch[1], Franz Ahlers[1], Thomas Weimann[1], and •Andrey Turchanin[2] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [2]Faculty of Physics, University of Bielefeld, 33615 Bielefeld, Germany

Chemical functionalization of single-layer graphene (SLG) is of key importance for implementations of this material in functional electronic devices such as, e.g., field effect transistor (FET) based nanosensors. However, the electronic quality of graphene typically degrades after the functionalization with presently employed methods, significantly restricting the application areas. Here, we present a route to non-destructive chemical functionalization of graphene via engineering of carbon nanomembrane (CNM)/SLG hybrids. We employ SLG, grown by methane CVD on Cu foils, and amino-terminated 1 nm thick CNMs, generated by electron-beam-induced crosslinking of aromatic self-assembled monolayers, to fabricate hybrid CNM/SLG FETs on oxidized silicon wafers. Structural, chemical and electronic properties of these devices are characterized by Raman spectroscopy, X-ray photoelectron spectroscopy and electrical transport measurements. We unambiguously show that the intrinsically high electronic quality of pristine SLG is preserved in the amino-functionalized hybrids opening broad avenues for their use in graphene-based FETs.

O 91.4 Fri 11:15 H17

Etching Nanoscale tunnels into graphite- a new route to produce suspended graphene — •Maya Lukas[1], Velimir Meded[1], Aravind Vijayaraghavan[1,2], Li Song[3,4], Pulickel M. Ajayan[4], Karin Fink[1], Wolfgang Wenzel[1], and Ralph Krupke[1,5] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, D-76021 Karlsruhe — [2]School of Computer Science, The University of Manchester, UK — [3]Research Center for Exotic Nanocarbons, Shinshu University, Nagano, Japan — [4]Department of Mechanical Engineering & Materials Science, Rice University, Houston, TX , USA — [5]Department of Materials and Earth Sciences, Technische Universität Darmstadt, D-64287 Darmstadt

Catalytic hydrogenation of graphite, although known since the 1970s, has recently attracted renewed attention, as a route for nanopatterning of graphene and to produce graphene nano-ribbons. These reports show that metallic nanoparticles etch surface layers of graphite or graphene anisotropically along the crystallographic zigzag <11-20> or armchair <1010> directions.

We report the sub-surface etching of highly oriented pyrolytic graphite (HOPG) by Ni nanoparticles, to form a network of tunnels, as seen by SEM and STM. The layers on top of tunnels which are only a few layers below the surface bend inward, while their local density of states remains fundamentally unchanged. Our work opens a new route to produce suspended graphene for the study of fundamental mechanical and electronic properties. M. Lukas, V. Meded *et al., Nat. Commun.* accepted for publication

O 91.5 Fri 11:30 H17

Direct e-beam writing of single-layer graphene nanostructures — •Nils-Eike Weber[1], Henning Vieker[1], Stefan Wundrack[2], Rainer Stosch[2], and Andrey Turchanin[1] — [1]Fakultät für Physik, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig

We demonstrate direct writing of single-layer graphene nanostructures employing electron irradiation of aromatic self-assembled monolayers (SAM) and subsequent annealing. The process consists of the following technological steps: (i) formation of an aromatic SAM on a Cu substrate; (ii) electron-beam-irradiation of the SAM resulting in locally cross-linked SAM areas; (iii) conversion of these areas into single-layer graphene via annealing. In this way graphene nanostructures of various architectures are directly defined in the SAM by electron beam lithography reducing several manufacturing steps, which are typically applied for the patterning of two-dimensional sheets including graphene (baking and developing electron-beam resist, plasma etching, resist striping). The formed nanostructures were characterized by Raman spectroscopy, scanning electron and helium ion microscopy. We demonstrate their successful transfer from the original copper foils onto oxidized silicon wafers, where they can directly be integrated into electronic devices.

O 91.6 Fri 11:45 H17

Understanding of the imaging contrast in STM/NC-AFM of graphene on metals — •Elena Voloshina[1], Edoardo Fertitta[1], Andreas Garhofer[2], Florian Mittendorfer[2], Mikhail Fonin[3], Torben Haenke[4], Oliver Schaff[4], Thorsten Kampen[4], Andreas Thissen[4], and Yuriy Dedkov[4] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institute of Applied Physics, Vienna University of Technology, Gusshausstr. 25/134, 1040 Vienna, Austria — [3]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [4]SPECS Surface Nano Analysis GmbH, Voltastraße 5, 13355 Berlin, Germany

Realization of graphene moiré superstructures on the surfaces of 4d and 5d transition metals offers templates with periodically modulated electron density, which is responsible for a number of fascinating effects, including the formation of quantum dots and the site selective adsorption of organic molecules or metal clusters on graphene. Here, applying the combination of scanning probe microscopy/spectroscopy and the density functional theory calculations, we gain a profound insight into the electronic and topographic contributions to the imaging contrast of the epitaxial graphene/Ir(111) system. We show directly that in STM imaging the electronic contribution is prevailing compared to the topographic one. In the force microscopy and spectroscopy experiments we observe a variation of the interaction strength between the tip and high-symmetry places within the graphene moiré supercell, which determine the adsorption sites for molecules or metal clusters on graphene/Ir(111).

O 91.7 Fri 12:00 H17

Precise imaging of graphene — •Thomas Hofmann, Alfred J. Weymouth, Joachim Welker, and Franz J. Giessibl — Institut für Experimentelle und Angewandte Physik, Universität Regensburg

Atomic imaging of graphene with a scanning probe microscope is challenging due to its small atomic lattice. We show that metallic tips, which have been characterized prior to the measurement, cannot truthfully image the graphene surface due to their large, non-spherical electron density [1]. Calculations predict that the metal tip atom strongly interacts with the graphene surface [2]. Carbon oxide front atom identification (COFI) [2] shows that contact of a clean metal tip with graphene can lead to graphene flakes attaching to the tip apex. This results in blurred images and multi-valley force versus distance curves. As a solution we use a metal tip, functionalized with an inert carbon monoxide molecule as suggested by Gross et al. [3]. The closed-shell nature of the CO drastically reduces the attraction between tip and graphene. Additionally, the small size of the CO allows truthful imaging of the graphene surface.

[1] *J. Welker, and F. J. Giessibl, Science 336, 6080 (2012)

[2]*M. Ondráček, P. Pou, V. Rozsíval, C. González, P. Jelínek, and R. Pérez, PRL 106, 176101 (2011)

[3]*L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, Science 325, 5944 (2009)

O 91.8 Fri 12:15 H17

Role of substrate-molecular interactions in arrangement and collective motion of fullerene islands on graphene — •Martin Svec[1], Pablo Merino[2], Yannick Dappe[3], Cesar Gonzalez[1], Enrique Abad[4], Pavel Jelinek[1], and Jose-Angel Martin-Gago[5] — [1]Institute of Physics, ASCR, Prague, CZ — [2]CAB INTA-CSIC, Madrid, ES — [3]CEA, IRAMIS, SPCSI, FR — [4]UAM, Madrid, ES — [5]ICMM-CSIC, Madrid, ES

Fullerenes interacting with graphene are a model system, that should be entirely driven by van der Waals (vdW) interactions. We concentrate on the interactions occurring between fullerenes and the single-layer graphene grown on SiC(0001) [1]. By using a VT-STM at 40K, regular islands of fullerenes were found. The particular orientation of the fullerenes in the islands, which occupy 4x4 graphene unit cells each, is critically evaluated by a comparison of STM measurements to extensive STM simulations with realistic fullerene-terminated tips. The determined orientation of fullerenes is independently confirmed by complex theoretical calculations of several adsorption configurations, taking into account the vdW interaction between the constituents of this system. Furthermore, islands of fullerenes were found collectively moving on the graphene. Surprisingly, according to the theory, the cohesion among the fullerenes is weaker than adhesion to the surface. Nevertheless, cohesion is a decisive factor in the collective motion, thanks to a low diffusion barrier of fullerenes on graphene.

[1] M. Švec et al., Phys. Rev. B 86 121407(R)(2012)

O 91.9 Fri 12:30 H17

XPS Analysis of Wet-Chemically Prepared Graphene Oxide — •Ole Lytken, Michael Röckert, Jie Xiao, Christian Papp, Hans-Peter Steinrück, Siegfried Eigler, Michael Enzelberger, Stefan Grimm, Philipp Hofmann, Wolfgang Kroener, Christoph Dotzer, Paul Müller, and Andreas Hirsch — Universität Erlangen-Nürnberg

Graphene is one of the most studied materials of the last few years, but large scale production of high-quality graphene remains a challenge. One approach to a large scale production of graphene is the oxidation of graphite to graphite oxide, which can be exfoliated to graphene oxide and subsequently reduced to graphene. The challenge of this method is to keep the carbon structure intact during oxidation. We report on the XPS analysis of graphene oxide produced by a mild synthesis method that keeps the carbon structure intact and allows the reduction back to high-quality graphene. Only carbon with a single bond to one neighboring oxygen atom is observed (e.g. alcohols, expoxides or ethers), but no carbonyl (C=O) or carboxyl (-COOH) groups are found. Some common problems related to the interpretation of graphene oxide XPS spectra in the presence of charging and sulfur impurities will be touched upon.

Support by the SFB 953 and the Alexander-von-Humboldt Foundation is gratefully acknowledged.

O 91.10 Fri 12:45 H17

Morphological and Electronic Study of Moirê Patterns due to Dislocated Graphene on HOPG — •Dilek Yildiz[1], Şener Şen[2], Oğuz Gülseren[2], and Oğuzhan Gürlü[1] — [1]Istanbul Technical University, Istanbul, Turkey — [2]Bilkent University, Ankara, Turkey

Highly oriented pyrolytic graphite (HOPG) is widely used as a calibration sample for scanning tunneling microscopy (STM) studies. It is also used as a substrate in surface science because of its smooth surface. HOPG is composed of stacked two dimensional hexagonal lattices formed by carbon atoms, popularly named as graphene layers. Because of the weak van der Waals bonding between the graphene layers, the topmost layer may be shifted or rotated on HOPG. Due to the rotation of the top layer, super-periodic structures called as Moiré patterns form on HOPG. These formations were investigated in numerous studies; however, they are rediscovered in graphene research and their origin is still not understood. In this study we used different solvents to see their effects on HOPG samples and the formation of super-periodic structures on these surfaces. We investigate the morphological and electronic properties by using scanning tunneling microscopy and spectroscopy (STM and STS) under ambient conditions. We compared electronic properties of Moiré patterns due to their periodicities. In order to shed light onto the observed electronic structures we also performed ab initio calculations on these super periodic structures. (Supported by TUBITAK 109T687 and ITU-BAP 33263).

O 92: Invited Talk (Helmut Zacharias)

Time: Friday 13:15–14:00 Location: H36

Invited Talk O 92.1 Fri 13:15 H36

Room-temperature electron spin filtering by ordered thin films of helical organic molecules — •Helmut Zacharias — Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Since more than a decade the manipulation of the electron spin is considered as a method to facilitate electronic operations, so-called spintronic devices. Recently, the transmission of low-energy photoelectrons through ordered self-assembled layers of chiral molecules has been studied, showing an intensity dichroism for the two circular polarizations. This observation has been interpreted as a spin-dependent transmission through these ordered layers. We extend these studies by directly measuring the electron spin polarization using a calibrated Mott detector. For ordered layers of double-stranded oligo-DNA on gold and at room temperature a significant spin orientation is observed, even for linearly polarized light, ranging from about -8% for 26 base-pair (bp) DNA to -57% for 78 bp DNA [1]. The order of the self-assembled monolayer is very important for the spin filtering effect. Using further magnetized Ni as substrate to inject spin-polarized electrons into attached oligo-DNA of the same type as used in the photoemission experiment also a spin-dependent conductance through the helical molecules is observed [2]. First model calculations yield results which are qualitative in agreement with the experiment.

[1] B. Göhler et al., Science 331, 894 (2011); [2] Z. Xie et al., Nano Lett. 11, 4652 (2011)